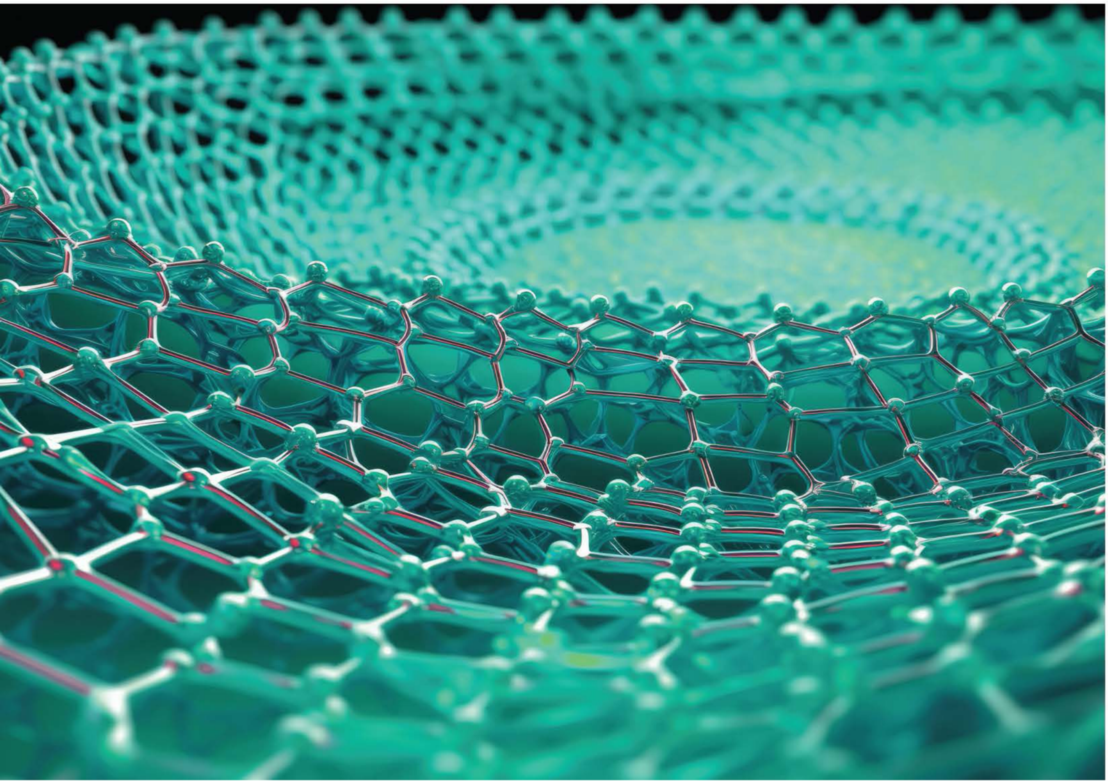
Frontiers of Mechanical and Industrial Engineering

Smart Materials and Applications



Kamal Kumar Kushwah | Shilpi Jindal | Ajay Kumar Vyas | Prasenjit Chatterjee
Editors

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SMART MATERIALS AND APPLICATIONS

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Kamal Kumar Kushwah, PhD

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Editors

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DEDICATION

The Editors would like to dedicate this book
to their parents, life partners, children, students,
scholars, friends, and colleagues.

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CONTENTS

Contributors .... *xiii*

Abbreviations .... *xvii*

Preface .... *xix*

Acknowledgment .... *xxv*

PART I: Introduction to Smart Materials 1

1. Emerging Frontiers: Harnessing the Potential of Smart Materials 3
Meenu Rani, Y. P. Singh, Sheela Devi, Shilpi Jindal, and Amit Kumar

2. Classification of Smart Materials 27
Naveen Bansal and Shivani Singla

3. Exploring the Potential of Smart Materials: An Overview of Properties and Applications 53
R. Padmavathi, C. Gladis Raja Malar, P. Rekha, and V. Kanchana

4. Graphene-Based Materials for Solar Cells: Review 73
Arti Sharma, Pragyan Jain, R.S. Rajput, Sunil Kumar, Prabhat Patel, and R. Bajpai

5. Fabrication Techniques of Smart Materials 95
Nupur Aggarwal, Anu Kapoor, Naveen Kumar, and Anjana Sharma

PART II: Classification of Smart Materials 121

6. Machine Learning for Smart Material 123
Hameed Khan, Kamal Kumar Kushwah, Jitendra Singh Thakur, Rajesh Tiwari, Gireesh Gaurav Soni, and Kishor Kumar Sadasivuni

7. Impact of Smart Materials on Digital Twin 143
Saweta Verma, Sonia Bajaj, and Garima Chandel

8. Deep Learning Methods in Material Science 171
Anjana Sharma, Shivam, Naveen Kumar, and Shilpi Jindal

9. Nature-Based Smart Materials (NBSMs): Properties, Types, and Applications 203
Anamika Roy

10. Review on Dye-Sensitized Solar Cells (DSSCs): Smart Material for Renewable Energy....227
Ankit Kargeti, Shamoon Ahmad Siddiqui, and Tabish Rasheed

11. Using Lime Water in the Manufacturing of Ferrochrome Ash-Based Geopolymer Concrete....243
Jyotirmoy Mishra, Bharadwaj Nanda, Sanjaya Ku. Patro, R. S. Krishna, Shaswat Ku. Das, and Syed M. Mustakim

PART III: Applications of Smart Materials....265

12. Trends in Robotics Technology: Solution for Materials to Manufacturing....267
Sonia Bajaj, Garima Chandel, Gyanendra Singh, Lakshay Sharma, Aryan Wagh, and Arjun Krishna

13. Role of Smart Materials in the Adaptation of Electric Vehicles....291
Rupesh Kushwah, R. K. Pathak, Rakhi Khabiya, and Pratibha Sharma

14. Rheology of Smart Materials in Science and Engineering Fields: An Industrial Perspective....313
V. Renuga

15. Impact of Materials in Solar Photovoltaic Applications in Standalone System....337
Raj Jadav, Vandit Shah, Krutarth Patel, Shivang Shah, and Alok Kumar Singh

16. 4D Printing: Fundamentals, Materials, Applications and Challenges...359
Kamaldeep Kaur and Arashdeep Singh

17. Smart Materials for Healthcare....381
Kirti Vishwakarma and Om Prakash Vishwakarma

18. Binary Chalcogenide Polymer Nanocomposites for Electroluminescence and Photovoltaic Solar Cell Applications....403
Swati Dubey, Kamal Kumar Kushwah, Parveen Ansari, Hussain Jeevakhan, Sarita Kumari, Nitendra Gautam, and Meera Ramrakhiani

Index....427

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ABBREVIATIONS

3DP	3D printing
AI	artificial intelligence
AM	additive manufacturing
APT	active property tuning
ASET	active strain energy tuning
ASM	active smart material
CBD	chemical bath deposition
CFRPs	carbon fiber-reinforced polymers
CNT	carbon nanotube
CVD	chemical vapor deposition
DL	deep learning (DL)
DIW	direct ink writing
EAPs	electroactive polymers
EEC	elastic electric cable
EL	electroluminescence
EPD	electrophoretic deposition
ER	electrorheological
EVs	electric vehicles
FDM	fused deposition modeling
FTO	fluorine-doped tin oxide
GN	graphene
ML	machine learning
MEMS	microelectromechanical systems
MPPT	maximum power point tracking
MR	magnetorheological
MRF	magnetorheological fluid
NN	neural network
NPs	nanoparticle
PCMs	phase change materials
PL	photoluminescence
PSM	passive smart material
PSO	particle swarm optimization
PV	photovoltaic
PVA	polyvinyl alcohol

PWM	pulse width modulation
rGO	reduced graphene oxide
SAM	shape memory alloy
SEM	scanning electron microscopy
SLA	stereolithography
SLM	selective laser melting
SMA	shape memory alloys
SMAF	shape memory alloy fibers
SME	shape memory effect
SMPs	shape memory polymers
SMs	smart materials
SVM	support vector machines
TFSC	thin film solar cell
XRD	X-ray diffraction

PREFACE

Smart materials, often referred to as intelligent or responsive materials, possess unique properties that enable them to respond to external stimuli such as temperature, pressure, light, or magnetic fields. They can change their physical or chemical characteristics in a controlled and predictable manner, making them invaluable for solving complex engineering challenges and driving innovation in science and technology.

The concept of smart materials has been around for decades, but recent advancements in materials science and nanotechnology have opened up new possibilities that were once considered science fiction. Today, these materials are at the forefront of scientific research, engineering, and design, with applications spanning fields as diverse as aerospace, healthcare, energy, and consumer electronics.

This book is intended to serve as a comprehensive 18 chapters and will be a resource for students, researchers, engineers, and professionals interested in understanding the principles and applications of smart materials. It is structured to provide a clear and accessible introduction to the fundamentals of smart materials, followed by in-depth discussions of their applications in various domains.

Chapter 1 presents a comprehensive understanding of these materials and the extraordinary ways they respond to external stimuli. Smart materials, often described as intelligent or responsive materials, possess the exceptional ability to adapt and transform in response to changes in their environment. Their properties can be harnessed and controlled, making them invaluable for a wide array of applications across multiple industries. From shape-shifting alloys to materials that generate electricity from mechanical stress, the possibilities presented by smart materials are nothing short of revolutionary.

Chapter 2 embarks on a journey to classify and explore the diverse world of smart materials, each category a testament to the ingenuity of scientists and engineers in harnessing nature's secrets to develop materials with extraordinary capabilities. Smart materials, often referred to as intelligent or responsive materials, have the remarkable ability to respond to external stimuli in a predictable and controlled manner. They are the building blocks of transformative technologies that have found applications in an array of industries, from healthcare to aerospace, and from energy to consumer electronics.

Chapter 3 delves into the fundamental properties that define smart materials, including shape memory, piezoelectricity, and magnetostrictive, among others and explores the underlying science and engineering principles that enable these materials to exhibit such unique behavior. From shape-shifting alloys to self-healing polymers, the capabilities of smart materials continue to expand, offering a wide array of possibilities for applications across various industries. Moreover, the diverse range of applications where smart materials have already made a significant impact and are poised to revolutionize the future. From the aerospace and automotive industries to healthcare and consumer electronics, these materials are finding their way into an increasing number of products and systems, enhancing functionality, efficiency, and safety.

Chapter 4 provides an insightful overview of the recent advances in graphene-based materials and their pivotal role in photovoltaic applications. As we embark on this journey through the exciting realm of smart materials in the context of renewable energy, we invite you to explore the remarkable progress and immense potential that lie ahead. Graphene, a single layer of carbon atoms arranged in a hexagonal lattice, has captivated the scientific community since its isolation in 2004. Its extraordinary electrical, mechanical, and optical properties have paved the way for revolutionary developments in various domains of science and technology, with photovoltaics being a particularly promising frontier. This chapter serves as a window into the world of graphene-enabled materials, shedding light on their unique attributes and their impact on the future of solar energy harvesting.

Chapter 5 explores the fascinating world of fabrication techniques, each tailored to harness the unique properties of smart materials. Whether it's the precision of nanofabrication for creating miniature sensors or the artistry of 3D printing for crafting complex structures, & also explore the processes that transform raw materials into functional, responsive systems. The potential of smart materials and their fabrication techniques is boundless, and the breakthroughs and innovations that will shape the materials landscape for the next generations.

Chapter 6 aims to provide a comprehensive overview of how machine learning is revolutionizing the smart materials landscape. The theoretical foundations of machine learning and its integration into the study of smart materials as well as cutting-edge research, real-world applications, and the challenges that lie ahead in harnessing the power of data-driven insights.

Chapter 7 is designed to serve as a valuable resource for researchers, engineers, digital twin enthusiasts, and all those intrigued by the possibilities that emerge when the physical and digital worlds seamlessly merge. this chapter provides a deeper understanding of the revolution taking place in materials science and digital technology. Simultaneously, the concept of the digital twin has evolved to create virtual representations of real-world objects, systems, and processes.

Chapter 8 provides an extensive exploration of deep learning's impact on materials science. Also delve into the depths of neural networks, and machine learning algorithms, and explore their versatile applications in predicting material properties, analyzing complex structures, and facilitating high-throughput materials screening & investigate the fundamental concepts, methodologies, and applications that empower researchers to harness the incredible potential of data-driven insights.

Chapter 9 is dedicated to exploring the diverse and captivating realm where biomaterials, inspired by nature's design, intersect with the evolving landscape of smart materials and their applications. In the pursuit of sustainable and biocompatible materials, nature has long been a source of inspiration. The genius of evolution has crafted materials with remarkable properties, adaptability, and intelligence, offering a blueprint for the biomaterials of the future. With a keen focus on ecological sustainability, these materials provide a unique bridge between the natural world and human-made technology.

Chapter 10 is based on dye-sensitized solar cells representing a remarkable marriage of materials science, photonics, and renewable energy technology. With the promise of harnessing sunlight efficiently and economically, the potential to revolutionize our global energy landscape. These smart materials mimic the photosynthetic processes of nature, capturing light and converting it into electrical energy with remarkable efficiency.

Chapter 11 provides a comprehensive overview of the utilization of Ferrochrome ash in geopolymer concrete production, with a particular focus on the role of lime water. We delve into the principles and chemistry behind this innovative material, exploring its potential applications and the sustainable practices it represents. The convergence of geopolymer technology, waste recycling, and concrete production has emerged as an exciting frontier in the construction industry.

The objective of Chapter 12 is to provide an in-depth exploration of the latest trends in robotics technology and their applications in materials science and manufacturing. In an era of rapid technological advancement, robotics technology stands as a driving force in the transformation of manufacturing processes and materials handling. These intelligent machines are at the heart of the fourth industrial revolution, reshaping industries, enhancing efficiency, and unlocking new possibilities across a wide array of sectors.

Chapter 13 is designed to serve as a valuable resource for automotive engineers, researchers, environmentalists, and all those captivated by the intersection of smart materials and sustainable transportation. Electric vehicles (EVs) are emerging as a sustainable and environmentally responsible solution to the challenges of urbanization and climate change. Within this profound shift, the integration of smart materials is redefining the capabilities, safety, and efficiency of electric mobility.

Chapter 14 is intended to serve as a valuable resource for industrial professionals, researchers, engineers, and all those intrigued by the convergence of smart materials and rheology. Rheology, the study of the flow and deformation of matter, is a fundamental science with far-reaching applications. When combined with the remarkable properties of smart materials, it offers an intriguing window into the future of materials science, manufacturing, and countless other fields.

Chapter 15 provides an overview of how materials influence solar photovoltaic applications in standalone systems. Also describe principles, technologies, and materials that have the power to optimize energy capture, storage, and delivery. From advanced solar cell materials to innovative energy storage solutions, materials science is shaping the future of solar energy. Solar photovoltaic technology has become a cornerstone of the global effort to transition to sustainable and renewable energy sources. As the demand for clean energy continues to rise, the quest for materials that can enhance the performance of photovoltaic systems has gained significant momentum.

Chapter 16 based on 4D printing represents a significant leap forward in the field of advanced manufacturing. It combines the principles of 3D printing with materials that respond to environmental stimuli, such as temperature, humidity, or light, to create objects that can self-assemble, self-repair, or undergo shape-shifting transformations. The potential applications of 4D printing are vast, spanning industries as diverse as aerospace, healthcare, and architecture.

Chapter 17, Smart Material for Healthcare, stands on the cusp of a remarkable transformation, driven by the convergence of cutting-edge materials science and the growing demands for improved medical solutions. Smart materials, with their unique properties and responsiveness, offer an array of opportunities to enhance diagnostics, treatments, and patient care.

Chapter 18 explores "Binary Chalcogenide Polymer Nano-composites for Photovoltaic—Solar Cell Applications" and discovers the transformative potential these materials hold in the quest for cleaner and more efficient energy production. The global pursuit of clean and sustainable energy sources has made photovoltaic technology one of the cornerstones of our renewable energy landscape. In this context, the emergence of binary chalcogenide polymer nanocomposites as a materials solution is both promising and exciting. These nanomaterials bring unique properties that have the potential to revolutionize solar cell design and efficiency.

Editors
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—The Editors

PART I

Introduction to Smart Materials

CHAPTER 1

EMERGING FRONTIERS: HARNESSING THE POTENTIAL OF SMART MATERIALS

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ABSTRACT

Smart materials belong to a class of materials which is enlisted in advanced materials. They are also known as intelligent materials. Smart materials are increasingly gaining popularity in modern society due to their crucial role and unique properties, surpassing traditional materials. These materials are capable of adapting to their environment by reacting intelligently to external stimuli. They can adjust to specific triggers and can be categorized in various ways, such as different types of responses to environmental stimuli including physical, chemical, and biological stimuli. Many smart materials, such as piezoelectric materials and shape memory alloys, are currently in

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use, with new discoveries expected as a result of ongoing intensive research and development efforts. Smart materials are utilized in a variety of sectors such as medical, robotics, nuclear power, military, aerospace technology, civil engineering, construction, general industries, biomedical industries, and seismic applications. These materials offer inherent properties such as sensing, information processing capabilities, control, and actuation, allowing for the creation of smart systems with multifunctional components. They are equipped with features like self-restoration, self-degradation, and self-diagnosis; thus enhancing their functionality. This chapter explores different types of smart materials with their properties and applications across various industries.

1.1 INTRODUCTION

Materials have been used by human beings for many different purposes for thousands of years, and this use of various types of materials has brought about many changes in the way of living their lives. The discovery of new types of materials has also become a basis for the classification of civilizations. The Stone Age was succeeded by the Bronze Age, a period that proved to be even more revolutionary thanks to two key properties of bronze—its durability and superior hardness compared to other materials of the time. The discovery of bronze marked the beginning of metallurgical processes that enabled humans to extract and utilize a wide range of new materials for various purposes [1]. Over the last two decades, science and technology have greatly contributed to the development of new materials, meeting the needs of the modern world. These new materials can be classified into four groups: ceramics, metals, polymers, and the smart materials [2]. Smart materials have been gaining increased popularity due to their extensive applications and unique properties compared to other material types. These smart materials are also called advanced materials or the intelligent materials. The development of smart materials is thought to be an answer to ever increasing demand for modern industrial, commercial, aeronautical, military, and biomedical applications. Advanced materials are attracting the attention of a lot of researchers worldwide. The word “smartness” refers to their sharp, active, and clever response and their multiple functionalities. They can change their properties in a particular manner when they are exposed to some external stimuli. They have got high level of functionality such as self-healing, self-degradation, sensing, and so many others. With the ability to detect changes in their environments, intelligent materials can then react to these changes in a predetermined manner. To respond to the physical changes like temperature, hydrostatic pressure, magnetic field, mechanical stress, strain, electric current, and chemical changes, they bring modification in their size, moisture, color, scent, and the viscosity of flow [3]. The characteristics such as noise, vibration, and so on of different materials and systems can be controlled in a simplified way by using smart materials. Many smart materials are already available and many more are to be discovered in near future as a result of intense research being done on them. This chapter provides a detailed explanation of various smart materials and their unique properties, as well as their potential uses across a range of industries.

1.2 DEFINITION OF SMART MATERIALS

There is no unique definition of smart materials [4–7]. Smart materials are typically described as possessing the ability to remember different shapes and adjust to specific stimuli, or as materials that can intelligently react to changes in their surroundings [8, 9]. They are capable of detecting signals from their environment and autonomously performing tasks. There are certain key features of these materials that distinguish them from other conventional materials [8–12]. The distinguishing traits of these materials include selectivity, transiency, self-actuation, immediacy, shape changing, self-sensing, self-diagnostic, and self-healing. These attributes set these materials apart as special due to their predetermined response (selectivity), ability to respond to various stimuli (transiency), internal intelligence (self-actuation), quick response to external factors (immediacy), ability to change shape in response to stimuli (shape changing), automated detection of external stimuli (self-sensing), automated detection of defects (self-diagnostic), and ability to self-heal that means the remarkable ability of materials to repair themselves automatically in the event of damage. Consequently, smart materials give an opportunity of an active and smart response in a system that would not have been obtained in their absence.

1.3 CLASSIFICATION OF SMART MATERIALS

Smart materials can be classified into two main classes: Active and Passive [13, 14]. Passive smart materials are those that can transfer energy in some form, such as optical fiber, which allows the transmission of electromagnetic waves. Active smart materials, on the other hand, can be further categorized into two types. The first category is of those materials that bring about a change in their properties when they are exposed to external stimulus. An example of this is photochromatic glasses, which alter their hue upon exposure to sunlight. [15]. The second classification of active smart materials includes those that have the ability to convert one form of energy into another. This energy can be in the form of thermal, mechanical, optical, chemical, electrical, or nuclear energy. Examples of these materials include solar cells and LEDs. Solar cells are the photovoltaic cells that can change solar energy into the electrical energy. Conversely, LEDs have the ability to convert electric energy into light energy [16, 17]. Piezoelectric, pyroelectric, and ferroelectric materials also belong to this type as they also generate electric energy by converting other forms of energy [18]. Therefore, if a given energy will cause a change in structure or microstructure of material, then it is of the first type, and if the form of energy is converted without causing any change in structure, then it is of the second type active smart material [19].

1.4 TYPES OF SMART MATERIALS

Smart materials can be divided into the following types depending on the different kind of responses to external stimuli.

1. Shape memory alloys: They respond to temperature and pressure.
2. Piezoelectric materials: They respond to electricity and pressure.
3. Electrostrictive materials: They respond to electric field.
4. Magnetostrictive materials: They respond to magnetic field.
5. Chromic materials: They react with different kinds of stimuli.
6. Magnetorheological fluid: They react with magnetic field.
7. Electrorheological fluid: They react with the electric field.

Each of these types of smart materials will be discussed in detail in the following sections.

1.4.1 SHAPE MEMORY ALLOYS

Shape memory alloys (SMAs) are the most common type of smart materials. These are the smart materials that have at least two phases. During changes in temperature or stress, there will be a transition from one phase to another. The two phases involved are austenite and martensite. Austenite phase is stable at higher temperatures, while martensite phase is stable at lower temperatures. They have a unique characteristic that they can regain their original shape after deformation because of their ability of remembering their shape in austenite phase. Nickel–titanium (Ni–Ti) alloy system is the most powerful type of SMA that has been used widely for commercial applications [20]. This is due to its characteristics such as good mechanical behavior, easy processing, high resistivity toward corrosion, and biocompatibility. This system is also known as nitinol alloy system and titanium percentage in this system is about 45%–50%. Zinc–aluminum alloy system and copper–aluminum–nickel alloy system are the other examples of SMAs. But absence of titanium limits their performance as SMAs to lower level as compared to nitinol alloy systems. Some common SMA systems have been provided in Table 1.1 [21–23].

TABLE 1.1 Some Shape Memory Alloys Systems[21–23] ⏎

Alloy	Composition	Transformation Temperature, A_s, Range (°C)	Transformation Hysteresis
Ag–Cd	44/49 at Cd	−190 to −50	~15
Au–Cd	46.5/50 at Cd	30 to 100	~15
Cu–Al–Ni	14/14.5 wt.% Al 3/4.5 wt.% Ni	−140 to 100	~35
Cu–Al–Ni polycrystalline	Cu 82.4 wt.%- Al 13.5wt.%-Ni 4.1wt.%	149	~21
Cu–Al–Ni single crystal	Cu 82.4 wt.%-Al 13.5wt.%-Ni 4.1wt.%	157	~12
Cu–Sn	15 at.% Sn	−120 to 30	~10
Cu–Zn	38.5/41.5 wt.% Zn	−180 to −10	~10
Cu–Zn–X X=Si, Sn, Al	Small wt. % X	−180 to 200	~10

The utilization of these alloy systems is contingent upon the temperature range and several other physical parameters. The impact of variations in these parameters on properties has been thoroughly investigated. Some of these studies include addition of new materials to these binary alloy systems [24–30], mechanical treatment [31, 32], heat treatment [31, 33–39], improving surface [40] different cooling methods [41–45], and different techniques of preparation of samples [46–48].

SMAs are a class of smart materials that have attracted significant research interest and are of great utility in a number of fields because of their unique properties. SMA materials can regain their original shape after being deformed, making them ideal for utilization in a variety of applications, such as actuators, sensors, and medical devices. In the following sections, we will explore the manufacturing techniques, characteristics, and potential uses of SMAs.

1.4.1.1 MANUFACTURING METHODS OF SHAPE MEMORY ALLOYS

There are different techniques used for manufacturing of SMAs resulting in different properties of the product formed [49]. These techniques mainly include casting, powder metallurgy, and rapid solidification. Each of these techniques has its own advantages.

1.4.1.1.1 Casting

Casting is one of the most common methods used to manufacture SMAs. The process consists of melting the desired alloy composition in a crucible and then pouring it into a mold. The mold can be made of various materials such as graphite, steel, or sand.

The casting process allows for the manufacturing of complex shapes and large quantities of material. However, the process can lead to in the formation of unwanted phases, such as brittle intermetallic compounds, which can affect the material's properties.

1.4.1.1.2 Powder Metallurgy

Powder metallurgy is another common method used to manufacture SMAs. The process involves mixing the desired alloy composition in a powdered form and then compacting this powder into the required shape using a press or other forming methods. The compacted powder is then sintered in a furnace to form a solid material.

Powder metallurgy allows for the fabrication of a wide range of shapes and sizes, including complex shapes with fine details. It also allows for the production of high-purity materials with excellent mechanical properties. However, the process is typically more expensive than other methods, and the resulting material may have lower ductility and toughness.

1.4.1.1.3 Rapid Solidification

Rapid solidification is a process in which molten metal is cooled at a very high rate, typically in the range of millions of degrees Celsius per second. The process produces a material with a fine microstructure, which can result in unique characteristics like increased strength and ductility.

Rapid solidification can be achieved using various methods such as melt spinning, atomization, and quenching. Melt spinning involves melting the alloy and then spinning it onto a rotating wheel, which rapidly cools the metal. Atomization involves spraying molten metal through a nozzle and then rapidly cooling the droplets. Quenching involves dropping the molten metal into a cooling medium, such as water or oil.

Rapid solidification allows us to produce high-strength and the high-ductility materials with unique properties. However, the process can be expensive and difficult to control, and the resulting material may have lower thermal stability.

1.4.1.1.4 Other Methods

Other methods used to manufacture SMAs include extrusion, rolling, and wire drawing. Extrusion involves forcing the alloy through a dye to form a specific shape. Rolling involves passing the alloy through a set of rollers to form a sheet or plate. Wire drawing involves pulling the alloy through a dye to form a wire.

These methods allow us to produce specific shapes and sizes with excellent mechanical properties. However, they may be more expensive than other methods, and the resulting material may have limited ductility and toughness.

1.4.1.1.5 Postprocessing

After the material has been manufactured, it may undergo postprocessing to improve its properties. Common postprocessing methods include heat treatment, annealing, and cold working.

In heat treatment, materials are heated to a precise temperature and then cooled at a specific rate in order to achieve the desired microstructure and properties. Annealing involves heating the material to a specific temperature before slowly cooling it to reduce stress and enhance ductility. Cold working, on the other hand, involves deformation of the material at room temperature to enhance its strength and hardness.

1.4.1.2 PROPERTIES OF SHAPE MEMORY ALLOYS

Unique features of these smart materials are their thermoelasticity, high damping capacity, and super elasticity.

1.4.1.2.1 Thermoelasticity

SMAs undergo a phase transformation from austenite to martensite on decreasing the temperature, that is, on cooling. This transformation of phase is responsible for their capability of regaining their original shape. The transformation from austenite phase to twinned martensite phase does not occur at a specific temperature, but rather within a range of temperatures. This change occurs when materials in the austenite phase at high temperatures are cooled down. This change does not affect the macroscopic shape or size of the material. If an external stress is applied on twinned martensite structure then it is transformed into deformed martensite. This deformed structure can get back to its original austenite phase on increasing the temperature. This effect is known as shape memory effect (SME) [50–52]. SME is of two types: one-way SME and two-way SME. Response of SMAs under different physical conditions is as shown in Figure 1.1 [53].

In one-way SME, material regains its shape on heating only, while in two-way SME, shape can be regained on heating as well as on cooling. When we decrease the temperature of crystal structure in austenite phase, then this will start converting into twinned martensite phase at a temperature M_s known as martensite start temperature and the process of this change will be finished at a temperature below M_f, that is, martensite finish temperature. On application of external stress, this twinned martensite structure is distorted to form deformed martensite structure. This deformed structure will go back to austenite phase after the removal of applied stress and then increasing the temperature. This process will start at temperature A_s, austenite start temperature and will get completed at A_f, austenite finish temperature. This recovery of strain depends on the direction of process. The SMAs in which this process takes place are called one way SMAs. In one-way SMAs, there is only one original shape in austenite phase, while in two-way SMAs, there are two recoverable shapes, one in both austenite as well as martensite phases. So, there will be a transformation from austenite to deformed martensite phase on cooling and reverse transformation will take place on heating. SMAs showing this effect are known as two-way SMAs. Normally, one-way SME is referred to as SME and two-way SME is not very important. As there are different temperatures for start and finish of phases. This difference between the temperatures from 50% of martensite Phase to 50% of austenite phase is called temperature hysteresis as shown in Figure 1.2 [54].

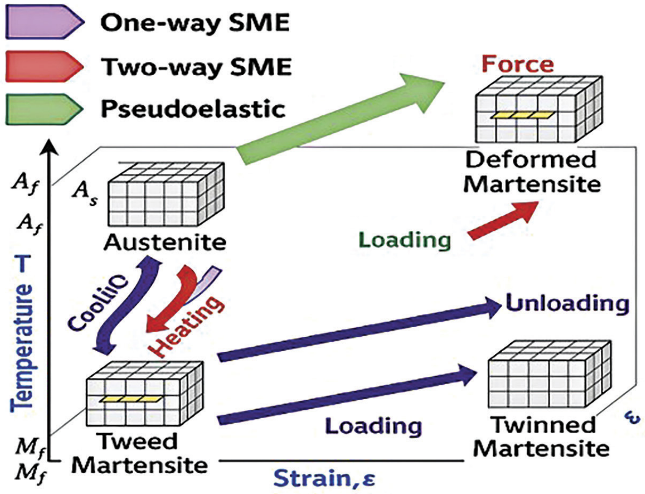
One-way SME
Two-way SME
Pseudoelastic
Force
Deformed Martensite
A_f
A_s
A_f
Austenite
Loading
Temperature T
CooliiC
Heating
Unloading
Twinned Martensite
Loading
M_f
M_f
Tweed Martensite
Strain, ε
ε

FIGURE 1.1 Schematic diagram of several shape memory effect for stress, strain, and temperature parameters [53]. ⏎

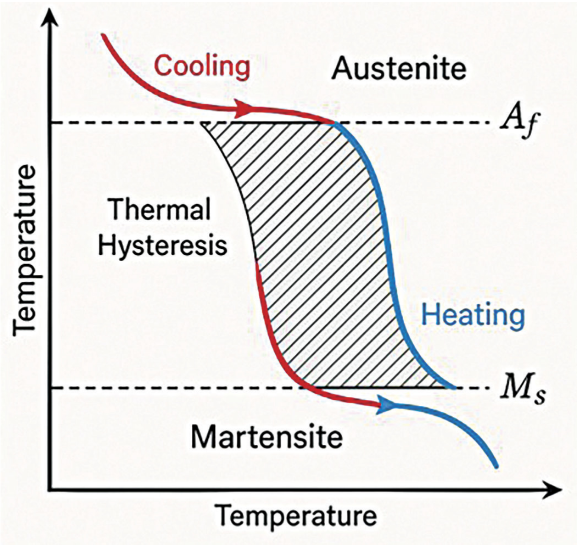
Cooling
Austenite
A_f
Temperature
Thermal Hysteresis
Heating
M_s
Martensite
Temperature

FIGURE 1.2 Phase transformation shape memory alloys. ⏎

1.4.1.2.2 Superelasticity

Superelasticity refers to an elastic response of SMAs when an external stress is applied on them. It is due to transformation of phase between austenite and martensite. But there is a difference between superelasticity and SME that the former occurs without a change in temperature while in the later, change of temperature is needed. It occurs at a temperature above A_f. At this temperature, there is the existence of a stable austenite phase. On application of an external force, austenite phase gets transformed into martensite phase and it is known as a stress induced martensite. This strain is held by affiliated shear of local regions. Now when the load is removed, the SMAs go back to their original austenite phase. During this transformation of phase, a fraction of energy will get consumed [55, 56]. Superelasticity is also known as pseudoelasticity.

1.4.1.2.3 Damping Capacity

Damping capacity can be defined as the tendency of the material to dissipate vibrational energy to the internal energy. SMAs possess high recovery of strain and therefore they will dissipate much greater energy as compared to steel or concrete [53, 57]. Damping capacity of material is affected by the amplitude of the vibration.

1.4.1.3 APPLICATIONS OF SHAPE MEMORY ALLOYS

Because of their unique characteristics, SMAs are used in a variety of applications. Some of these applications are as follows:

1.4.1.3.1 Actuators

SMAs are widely used in actuators because they are capable of changing their shape as a response to the external stimuli like temperature or mechanical load. Use of SMA actuators is done in fields such as robotics, aerospace, and the automotive industries. One of the advantages of SMA actuators is that they can provide a large force and displacement with a relatively low power input.

1.4.1.3.2 Medical Devices

SMAs are also used in medical devices such as stents, surgical tools, and orthodontic wires. The special properties of SMAs make them ideal for these applications. For example, SMA stents can be implanted in a compressed form, and then expanded in the body to the desired shape, reducing the invasiveness of the procedure. SMA orthodontic wires can apply a constant force on the teeth, resulting in a more comfortable and efficient treatment.

1.4.1.3.3 Sensors

SMAs are used in sensors because of their capability of changing shape as a result of response to external stimuli. For example, SMA strain gauges can measure changes in strain, and SMA temperature sensors can measure changes in temperature. SMA sensors have found applications in various industries such as aerospace, automotive industries, and the biomedical industries.

1.4.1.3.4 Smart Materials

SMAs are used as smart materials in various applications such as smart windows, smart fabrics, and smart composites. These materials can alter their properties in response to an external stimulus. For example, SMA smart windows can change their transparency in response to changes in temperature, and SMA smart fabrics can change their stiffness in response to changes in temperature.

1.4.2 PIEZOELECTRIC MATERIALS

The concept of piezoelectricity was discovered in the year 1880 by Pierre Curie and Jacques Curie during their study on quartz crystal, tourmaline, and the Rochelle salt. The word piezoelectricity is made up of two words: piezo and electricity. “Piezo” is a Greek word whose meaning is pressure. And second word “electricity” means electrical charges. When stress or strain is applied on a piezoelectric material, then it converts mechanical energy in the form of electrical energy and vice versa. The reason behind the piezoelectricity in materials is an asymmetry in its unit cell which gives rise to the connectivity between the mechanical distortion and the electric dipole separation. Piezoelectric effect is of 2 types: direct piezoelectric effect and inverse piezoelectric effect. In direct effect, a material is polarized and when a stress is applied on this material, the voltage will be produced. This stress can be either tensile or compressive in nature. The direction of polarization gets reversed according to the situation whether a tensile or compressive stress is applied [58]. This phenomenon is illustrated in Figure 3a [59, 60].

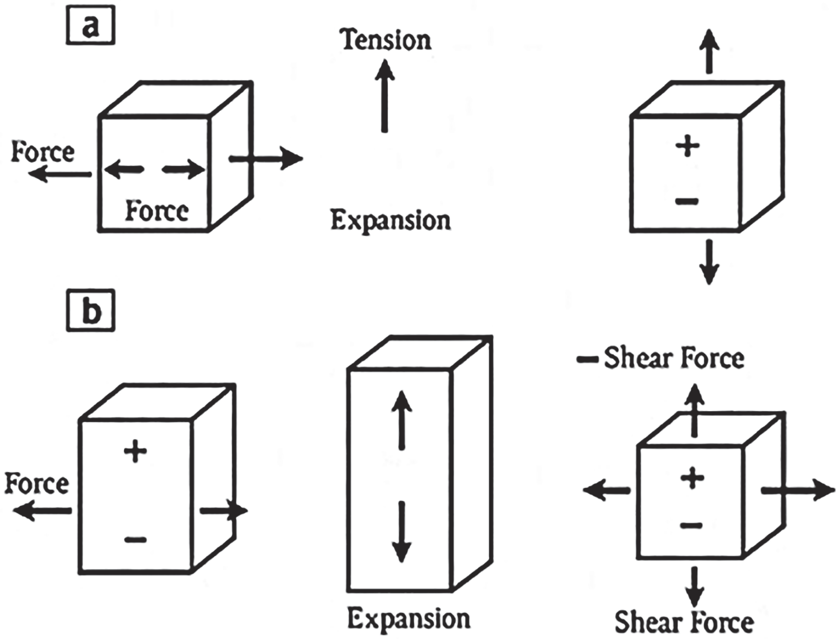

FIGURE 1.3 Schematic representation of piezoelectric effects. (a) Electric field produced by mechanical force, (b) change in shape on application of electric field in direction of polarization, and (c) production of shear force on application of electric field perpendicular to direction of polarization. ⏎

Figure 1.3b shows the reverse phenomena known as inverse piezoelectric effect that is on application of potential difference across piezoelectric materials, they will undergo a change in their size resulting in release of mechanical energy [61]. If we apply the potential difference in a direction orthogonal to direction of polarization of the piezoelectric material, then the bending of sample will take place as shown in Figure 1.3c and the direction in which bending occurs depends on the orientation of the material. These materials are of great use in a variety of applications. We just need to optimize their compositions in order to make them meet different requirements. For example, compositions with lead titanate help in obtaining high anisotropy while PMN-PT is relaxor having low value of hysteresis and high value of strain.

1.4.2.1 PIEZOELECTRIC SENSORS

The working of the sensors is based on direct piezoelectric effect. We can measure a lot of mechanical quantities directly by making use of piezoelectric materials. These quantities include torque, stress, acoustic sound, and so on. They have been categorized as part of the active smart materials because they do not require any external source as they are self-generating [62]. They are used for only instantaneous measurements. Other characteristics that make them special are their isolation to the electromagnetic radiations or the electric field and the magnetic field, high sensitivity [63], capability to operate over a large temperature range [64], and capacity to work in events involving high frequency [65–67].

1.4.2.2 PIEZOELECTRIC ACTUATORS

The working of these actuators is based on the inverse piezoelectric effect. In these, electrical energy is converted into mechanical energy, thus resulting in motion. The direction of orientation of crystal with respect to the direction of applied electric field will decide the direction of motion.

1.4.3 ELECTROSTRICTIVE MATERIALS

The materials which cause a change in their size as a response to the applied electric field are called as electrostrictive materials. This increase in size is due to displacement of ions from their original positions on applying electric field. The same feature is also exhibited by piezoelectric materials too but there are major differences between these two types of materials which are listed below:

- In electrostrictive materials, there is a nonlinear relationship between the change in size and the strength of the applied electric field [68]. While the same relationship is linear in case of piezoelectric materials [69].
- According to research [70], electrostrictive materials exhibit a consistent increase in size regardless of the direction of the applied electric field. In contrast, piezoelectric materials can undergo expansion or contraction depending on the direction of the applied electric field [71].
- Hysteresis of electrostrictive materials is less than that of piezoelectric materials at room temperature. Moreover, there is strong variation in hysteresis with temperature in electrostrictive materials and it does not vary much in case of piezoelectric materials [70, 72].

1.4.4 MAGNETOSTRICTIVE MATERIALS

Magnetostrictive materials are those materials which undergo a change in their size on application of magnetic field. Thus, applied magnetic field can lead to either stretching or contraction of the material. But this stretching or contraction of magnetostrictive materials is independent of the direction of applied magnetic field. They can be classified as positive or negative materials. Figure 1.4 shows the behavior of a magnetostrictive material on applying a magnetic field [49].

Figure 1.4a shows the random orientation of magnetic domains in absence of applied magnetic field, that is, for $H_1 = 0$. On application of small magnetic field $H_2 > 0$, few magnetic domains reorient themselves in the direction of applied magnetic field thus resulting in small increase in size as shown in Figure 1.4b. Figure 1.4c shows further increase in size of sample on increasing the value of applied magnetic field $H_3 > H_2$ due to increase in number of magnetic grains with similar orientation. On further increasing the magnetic field $H_4 > H_3$, now all the magnetic domains orient themselves in the direction of applied magnetic field thus resulting in maximum increase in size of sample as shown in Figure 1.4d. Now the elongation of sample has reached to its saturation. Energy density of magnetostrictive materials is very high. They find use in engine mounting, damper, and sensors.

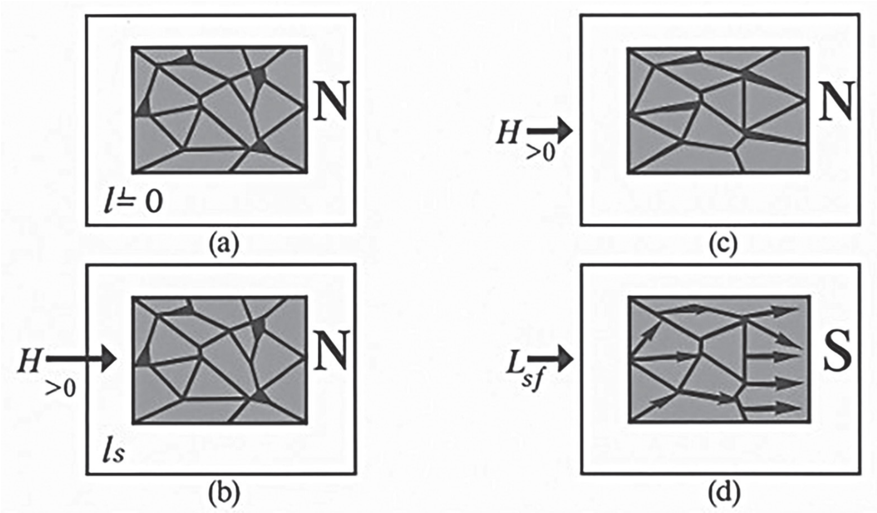

FIGURE 1.4 Schematic illustration of a positive magnetostrictive material in magnetic field, where $H_4 > H_3 > H_2 > H_1$. (a) In the absence of magnetic field $H_1 = 0$. (b) Elongation of ample at magnetic field H_2 (c) Continuation of expansion with increase in magnetic field, H_3. (d) Saturation of sample length at H_4. ⏎

1.4.5 CHROMIC MATERIALS

The materials which respond to the change in environmental conditions by bringing about a change in their color are known as chromic materials. When that change in environmental conditions is withdrawn, then they can regain back their original color. As this property is similar to the camouflage in chameleons hence these materials are also sometimes referred to as chameleon materials [73]. There are different groups of chromic materials depending upon the type of physical parameter to which response is to be given.

1.4.5.1 PHOTOCHROMIC MATERIALS

This group of chromic materials can absorb electromagnetic radiations like visible and UV radiations and then respond to them by giving some color depending on the intensity of the radiation absorbed. They can be organic as well as inorganic in nature. A very common example of these materials is photochromic eyeglasses [74].

1.4.5.2 THERMOCHROMIC

Thermochromic materials can change their color when we increase the temperature. This is because change in temperature brings about a change in the structure of the crystal or 3D positions of atoms. They are formed by metals, liquid crystals, and semiconductors. For example, use of thermostrips is done for making temperature indicators.

1.4.5.3 ELECTROCHROMIC

The materials in which the color is altered as a result of response to electrical voltage are known as electrochromic materials. This effect is because of transition of metal oxides [75] in some polymers and due to separation of positive charge and electrons in inorganic materials. Few devices based on electrochromic effect are electrochromic glass, electrochromic window, and so on.

1.4.5.4 MAGNETOCHROMIC

The materials which can change their color in response to magnetic field are called as magnetochromic materials, for example, ferrofluids having particles in the range 5–10 nm [76]. On applying magnetic field, alignment of particles occurs in a regular fashion. Figure 1.5 shows behavior of magnetochromic film when different values of magnetic field are applied [77].

1.4.5.5 PIEZOCHROMIC

The materials which undergo a change in certain physical properties such as reflectivity, absorbability, transparency, or emissivity when specific pressure is applied are known as piezochromic materials, for example, Palladium change its color at a pressure higher than 1.4 GPa and a change from green color to red color is observed in $CuMnO_4$ at a pressure of 2.5 kbar. Figure 1.6 depicts change in color of a piezochromic material under the application of external load [78].

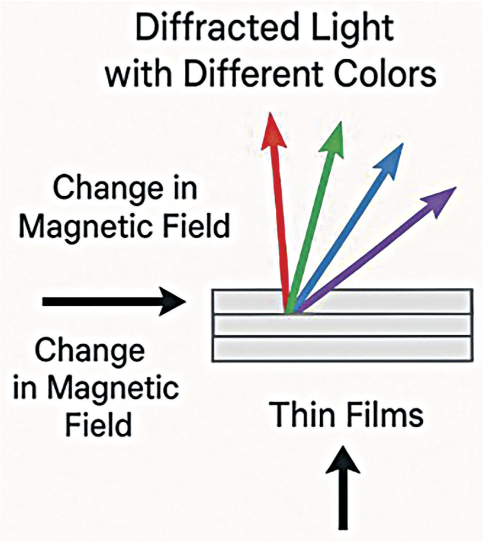
Diffracted Light
with Different Colors
Change in
Magnetic Field
Change
in Magnetic
Field
Thin Films

FIGURE 1.5 Change in magnetic field gives rise to diffracted light with different colors from films. ⏎

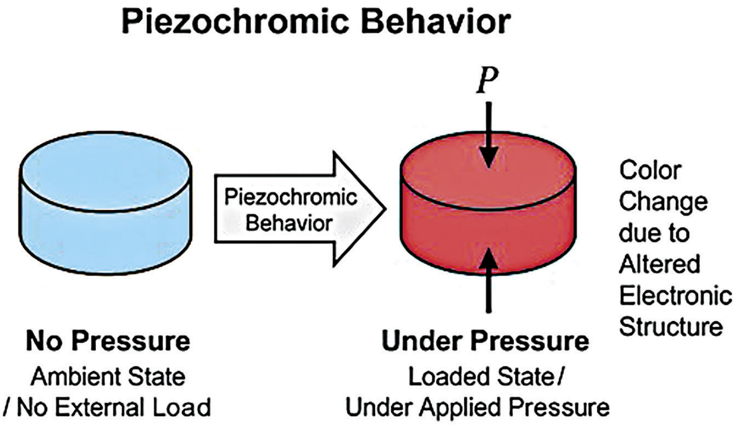
Piezochromic Behavior
P
Piezochromic
Behavior
Color
Change
due to
Altered
Electronic
Structure
No Pressure
Ambient State
/ No External Load
Under Pressure
Loaded State/
Under Applied Pressure

FIGURE 1.6 Change in color by applying pressure in piezochromic material. ⏎

1.4.5.6 pH SENSITIVE MATERIALS

These are the smart materials which respond to particular change in pH by altering color. They have a wide range of applications like in medical field for the purpose of delivering medicines [79] and can also act as filter [80].

1.4.6 MAGNETORHEOLOGICAL FLUIDS

These fluids are viscoelastic and come under the category of non-Newtonian fluids. They contain suspended particles. Under the application of magnetic field, they are capable of changing their viscosity as well as thickness. Size of microparticles in these fluids is about 0.1–10 µm. Figure 1.7 shows behavior of magnetorheological fluid in absence and presence of magnetic field [81]. Without external magnetic field, suspended particles are in disordered manner and on applying magnetic field, they align themselves in the direction of applied magnetic field. These fluids can help to protect the building during earthquake [82].

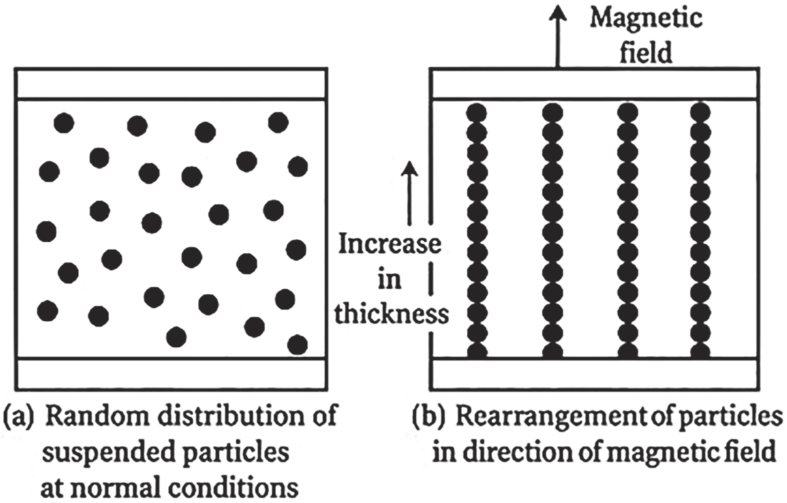
Magnetic field
Increase in thickness
(a) Random distribution of suspended particles at normal conditions
(b) Rearrangement of particles in direction of magnetic field

FIGURE 1.7 Schematic diagram of magnetorheological fluid. (a) Random distribution of suspended particles at normal conditions and (b) rearrangement of particles in direction of magnetic field and increase in thickness on applying magnetic field. ⏎

1.4.7 ELECTRORHEOLOGICAL FLUIDS

The materials exhibit similarities to magnetorheological fluids, with the key distinction being their consistent response to external electric fields. After their use for long time periods, these fluids become thick and then need to be replaced. They are used in vibration dampers hydraulic valves, shock absorber, and clutches.

1.5 CONCLUSION

Based on interdisciplinary field, the technology of smart materials is already in use in a number of industries but still a lot of potential related to this technology is yet to be discovered. After its maturity, this system will not only offer improved functionality, but it will also positively impact the environment by reducing material consumption and energy usage through extending the lifespan of the materials it produces. With their unique features, smart materials have got every potential to meet all the demand of changing world. No doubt, with intense research going on them, they will soon replace usual materials in many fields of applications without any failure.

KEYWORDS

- **smart materials**
- **advanced materials**
- **active and passive**
- **manufacturing methods**
- **applications**

REFERENCES

1. Levy, T.E., et al. Early bronze age metallurgy: a newly discovered copper manufactory in Southern Jordan. *Antiquity*, **2002**, *76*(292), 425–437.
2. Callister, W.D., Rethwisch, D.G. *Materials science and engineering: an introduction*. Vol. 7. John Wiley & Sons: New York, 2007.
3. Ward, M.A., Georgiou, T.K. Thermoresponsive polymers for biomedical applications. *Polymers*, **2011**, *3*(3), 1215–1242.
4. Takagi, T.A. Concept of intelligent materials and the current activities of intelligent materials in Japan. In *First European Conference on Smart Structures and Materials*, 1992, International Society for Optics and Photonics.
5. McCabe, J., et al. Smart materials in dentistry. *Aust. Dent. J.*, **2011**, *56*, 3–10.
6. Bogue, R. Smart materials: a review of recent developments. *Assem. Autom.*, **2012**, *32*(1), 3–7.
7. Hensel, M.U. Performance-oriented architecture and the spatial and material organisation complex. Rethinking the definition, role and performative capacity of the spatial and

material boundaries of the built environment. *FormAkademisk-forskningstidsskrift for design og designdidaktikk*, **2011**, *4*(1).

8. Addington, D.M., Schodek, D.L. *Smart materials and new technologies: for the architecture and design professions*. Routledge, 2005.
9. Addington, M., Schodek, D. *Smart materials and technologies in architecture: for the architecture and design professions*. Routledge, 2012.
10. Sadeghi, M.J., Masudifar, P., Faizi, F. The function of smart material's behavior in architecture. In *International Conference on Intelligent Building and Management*, LACSIT Press, 2011.
11. Mohamed, A.S.Y. Smart materials innovative technologies in architecture; towards innovative design paradigm. *Energy. Procedia.*, **2017**, *115*, 139–154.
12. Song, Y., Wei, W., Qu, X. Colorimetric biosensing using smart materials. *Adv. Mater.*, **2011**, *23*(37), 4215–4236.
13. Kamila, S. Introduction, classification and applications of smart materials: an overview. *Am. J. Appl. Sci.*, **2013**, *10*(8), 876.
14. Gautam, P., Valiathan, A. Bio-smart dentistry: stepping into the future! *Trends in Biomaterials and Artificial Organs*, **2008**, *21*(2), 94–97.
15. Ferrara, M., Bengisu, M. Materials that change color. In *Materials that change color*. Springer, 2014, pp. 9–60.
16. Parida, B., Iniyan, S., Goic, R. A review of solar photovoltaic technologies. *Renew. Sustain. Energy Rev.*, **2011**, *15*(3), 1625–1636.
17. Chang, M.-H., et al. Light emitting diodes reliability review. *Microelectron. Reliab.*, **2012**, *52*(5), 762–782.
18. Bai, Y., et al. Ferroelectric, pyroelectric, and piezoelectric properties of a photovoltaic perovskite oxide. *Appl. Phys. Lett.*, **2017**, *110*(6), 063903.
19. Vainstein, E. Smart materials and constructions. *Polym. Plast. Technol. Eng.*, **2001**, *40*(5), 703–714.
20. Buehler, W.J., Wang, F.E. A summary of recent research on the Nitinol alloys and their potential application in ocean engineering. *Ocean. Eng.*, **1968**, *1*(1), 105–120.
21. Huang, W. Shape memory alloys and their application to actuators for deployable structures. 1998.
22. Hautcoeur, A., Fouché, F. Sicre, J. Cu-Al-Ni shape memory single crystal wires with high transformation temperature. *Proceedings of the 43rd Aerospace Mechanisms Symposium*, NASA Ames Research Center, May 2016.
23. Smith, G. Photochromic glasses: properties and applications. *J. Mater. Sci.*, **1967**, *2*(2), 139–152.
24. Kök, M., et al., Examination of phase changes in the CuAl high-temperature shape memory alloy with the addition of a third element. *J. Therm. Anal. Calorim.*, **2018**, *133*(2), 845–850.
25. Ibrahim, M.K., Hamzah, E. Saud, S.N. Microstructure, phase transformation, mechanical behavior, bio-corrosion and antibacterial properties of Ti-Nb-xSn (x= 0, 0.25, 0.5 and 1.5) SMAs. *J. Mater. Eng. Perform.*, **2019**, *28*(1), 382–393.
26. Kök, M., Ateş, G. The effect of addition of various elements on properties of NiTi-based shape memory alloys for biomedical application. *Eur. Phys. J. Plus.*, **2017**, *132*(4), 185.
27. Ibrahim, M.K., et al. Effect of Sn additions on the microstructure, mechanical properties, corrosion and bioactivity behaviour of biomedical Ti–Ta shape memory alloys. *J. Therm. Anal. Calorim.*, **2018**, *131*(2), 1165–1175.

28. Ercan, E., Dagdelen, F., Qader, I. Effect of tantalum contents on transformation temperatures, thermal behaviors and microstructure of CuAlTa HTSMAs. *J. Therm. Anal. Calorim.*, **2019**, 1–8.
29. Dagdelen, F., Kok, M., Qader, I. Effects of ta content on thermodynamic properties and transformation temperatures of shape memory NiTi alloy. *Met. Mater. Int.*, **2019**, 1–8.
30. Kök, M., et al. The effects of cobalt elements addition on Ti2Ni phases, thermodynamics parameters, crystal structure and transformation temperature of NiTi shape memory alloys. *Eur. Phys. J. Plus.*, **2019**, *134*(5), 197.
31. Kök, M., et al. The change of transformation temperature on NiTi shape memory alloy by pressure and thermal ageing. In *Journal of Physics: Conference Series*, IOP Publishing, 2016.
32. Yang, C., et al. Effects of thermo-mechanical treatment on a Fe–30Mn–6Si shape memory alloy. *Mater. Sci. Eng.: A*, **2008**, *497*(1–2), 445–450.
33. Kök, M., Aydogdu, Y. Effect of heat treatment on the physical properties of Ni–Mn–Ga alloy. *Thermochim. Acta.*, **2012**, *548*, 51–55.
34. Dagdelen, F., et al. Influence of Ni addition and heat treatment on phase transformation temperatures and microstructures of a ternary CuAlCr alloy. *Eur. Phys. J. Plus.*, **2019**, *134*(2), 66.
35. Qader, I.N., Kök, M., Dağdelen, F. Effect of heat treatment on thermodynamics parameters, crystal and microstructure of (Cu-Al-Ni-Hf) shape memory alloy. *Physica B: Condens. Matter*, **2019**, *553*, 1–5.
36. Saedi, S., et al. The influence of heat treatment on the thermomechanical response of Ni-rich NiTi alloys manufactured by selective laser melting. *J. Alloys Compd.*, **2016**, *677*, 204–210.
37. Varzaneh, A.G., et al. Effect of heat treatment on martensitic transformation of Ni 47 Mn 40 Sn 13 ferromagnetic shape memory alloy prepared by mechanical alloying. *Met. Mater. Int.*, **2015**, *21*(4), 758–764.
38. Aydoğdu, Y., et al. The effects of thermal procedure on transformation temperature, crystal structure and microstructure of Cu-Al-Co shape memory alloy. In *Journal of Physics: Conference Series*, IOP Publishing, 2016.
39. Ozcan, H., et al. Effects of cyclic heat treatment and aging on superelasticity in oligocrystalline Fe-Mn-Al-Ni shape memory alloy wires. *Scr. Mater.*, **2017**, *134*, 66–70.
40. Firstov, G., et al. Surface oxidation of NiTi shape memory alloy. *Biomaterials*, **2002**, *23*(24), 4863–4871.
41. Saud, S.N., et al. Structure-property relationship of Cu-Al-Ni-Fe shape memory alloys in different quenching media. *J. Mater. Eng. Perform.*, **2014**, *23*(1), 255–261.
42. Saud, S.N., et al. Effects of quenching media on phase transformation characteristics and hardness of Cu-Al-Ni-Co shape memory alloys. *J. Mater. Eng. Perform.*, **2015**, *24*(4), 1522–1530.
43. Yildiz, K., Balci, E., Akpinar, S. Quenching media effects on martensitic transformation, thermodynamic and structural properties of Cu–Al–Fe–Ti high-temperature shape memory alloy. *J. Therm. Anal. Calorim.*, **2017**, *129*(2), 937–945.
44. Haidar, M.A., Saud, S.N., Hamzah, E. Microstructure, mechanical properties, and shape memory effect of annealed Cu-Al-Ni-xCo shape memory alloys. *Metallogr. Microstruct. Anal.*, **2018**, *7*(1), 57–64.
45. Dagdelen, F., Kanca, M.S., Boyrazli, M. Cooling condition effects on transformation temperature. *J. Chem. Technol. Metall.*, **2019**, *54*(1), 204–208.

46. Ibrahim, M.K., et al. Powder metallurgy fabrication of porous 51 (at.%) Ni–Ti shape memory alloys for biomedical applications. *Shape. Mem. Superelast.*, **2018**, *4*(2), 327–336.
47. Ibrahim, M.K., et al. Parameter optimization of microwave sintering porous Ti-23% Nb shape memory alloys for biomedical applications. *Trans. Nonferrous Met. Soc. China*, **2018**, *28*(4), 700–710.
48. Bahador, A., et al. Microstructure and superelastic properties of free forged Ti–Ni shapememory alloy. *Trans. Nonferrous Met. Soc. China*, **2018**, *28*(3), 502–514.
49. Kök, M., Qader, İ.N., Dağdelen, F., Aydoğdu, Y. Akıllı malzemeler üzerine derleme: araştırmalar ve uygulamaları. *El-Cezeri Fen ve Mühendislik Dergisi*. **2019**, https://doi.org/10.31202/ecjse.562177
50. Otsuka, K., Wayman, C.M. *Shape memory materials*. Cambridge University Press, 1999.
51. Watson, R.E. Comparison of the response of shape memory alloy actuators using air-cooling and water-cooling. Master's thesis, 1984.
52. Popescu, R., Popescu, D., Grumezescu, A. Applications of rubber-based blends, In *Recent developments in polymer macro, micro and nano blends*. Elsevier, 2017, pp. 75–109.
53. Jani, J.M., et al. A review of shape memory alloy research, applications and opportunities. *Mater. Des. (1980–2015)*, **2014**, *56*, 1078–1113.
54. Ozbulut, O.E., et al. Feasibility of self-pre-stressing concrete members using shape memory alloys. *J. Intell. Mater. Syst. Struct.*, **2015**, *26*(18), 2500–2514.
55. Choudhary, N., Kaur, D. Shape memory alloy thin films and heterostructures for MEMS applications: a review, Sens. *Actuat. A. Phys*., **2016**, *242*, 162–181, https://doi.org/10.1016/j.sna.2016.02.026.
56. Naresh, C., Bose, P.S.C., Rao, C.S.P. Shape memory alloys: a state of art review. *IOP Conf. Ser. Mater. Sci. Eng.*, **2016**, *149*, https://doi.org/10.1088/1757-899X/ 149/1/012054.
57. Pan, Q., Cho, C. The investigation of a shape memory alloy micro-damper for MEMS applications. *Sensors*, **2007**, *7*(9), 1887–1900.
58. Starr, M.B., Wang, X. Coupling of piezoelectric effect with electrochemical processes. *Nano. Energy*, **2015**, *14*, 296–311.
59. Anton, S.R., Sodano, H.A. A review of power harvesting using piezoelectric materials (2003–2006). *Smart. Mater. Struct.*, **2007**, *16*(3), R1.
60. Vatansever, D., Siores, E., Shah, T. Alternative resources for renewable energy: piezoelectric and photovoltaic smart structures. In *Global warming-impacts and future perspective*. IntechOpen, 2012.
61. Katsouras, I., et al. The negative piezoelectric effect of the ferroelectric polymer poly(vinylidene fluoride). *Nat. Mater.*, **2016**, *15*(1), 78.
62. Gautschi, G. Piezoelectric sensors. In *Piezoelectric sensorics*. Springer, 2002, pp. 73–91.
63. Algueró, M., et al. High-sensitivity piezoelectric, low-tolerance-factor perovskites by mechanosynthesis. *Chem. Mater.*, **2007**, *19*(20), 4982–4990.
64. Chang, Y., et al. ⟨001⟩ textured (K 0.5 Na 0.5)(Nb 0.97 Sb 0.03) O 3 piezoelectric ceramics with high electromechanical coupling over a broad temperature range. *Appl. Phys. Lett.*, **2009**, *95*(23), 232905.
65. Shung, K.K., Cannata, J., Zhou, Q. Piezoelectric materials for high frequency medical imaging applications: a review. *J. Electroceram.*, **2007**, *19*(1), 141–147.
66. Zhou, Q., et al. Piezoelectric films for high frequency ultrasonic transducers in biomedical applications. *Prog. Mater. Sci.*, **2011**, *56*(2), 139–174.
67. Li, H., et al. Fabrication of a high frequency piezoelectric microvalve. *Sens. Actuators. A Phys.*, **2004**, *111*(1), 51–56.

68. Newnham, R., et al. Electrostriction: nonlinear electromechanical coupling in solid dielectrics. *J. Phys. Chem. B.*, **1997**, *101*(48), 10141–10150.
69. Jaffe, B. *Piezoelectric ceramics*. Vol. 3. Elsevier, 2012.
70. Coutte, J., et al. Design, production and testing of PMN–PT electrostrictive transducers. *Ultrasonics*, **2002**, *40*(1–8), 883–888.
71. Yang, J. *An introduction to the theory of piezoelectricity*. Vol. 9. Springer Science & Business Media, 2004.
72. Davoudi, S. Effect of temperature and thermal cycles on PZT ceramic performance in fuel injector applications. Master's thesis, 2012.
73. Mattila, H. *Intelligent textiles and clothing*. Woodhead Publishing, 2006.
74. Akiyama, M., et al. Piezoelectric thin film, piezoelectric material, and fabrication method of piezoelectric thin film and piezoelectric material, and piezoelectric resonator, actuator element, and physical sensor using piezoelectric thin film. 2010, Google Patents.
75. Marinella, F., Murat, B. Materials that change color. *Smart materials, intelligent design*. Politecnico di Milano, Springer: Milano, 2013.
76. Sung, Y.K., Ahn, B.W., Kang, T.J. Magnetic nanofibers with core (Fe3O4 nanoparticle suspension)/sheath (poly ethylene terephthalate) structure fabricated by coaxial electrospinning. *J. Magn. Magn. Mater.*, **2012**, *324*(6), 916–922.
77. Horng, H.-E., et al. Magnetochromatic effects in magnetic fluid thin films. *Appl. Opt.*, **1998**, *37*(13), 2674–2680.
78. Seeboth, A., Loetzsch, D., Ruhmann, R. Piezochromic polymer materials displaying pressure changes in bar-ranges. *Am. J. Mater. Sci.*, **2011**, *1*(2), 139–142.
79. Chaturvedi, K., et al. Polymeric hydrogels for oral insulin delivery. *J. Contr. Rel.*, **2013**, *165*(2), 129–138.
80. Kocak, G., Tuncer, C., Bütün, V. pH-Responsive polymers. *Polym. Chem.*, **2017**, *8*(1), 144–176.
81. Park, B.J., Fang, F.F. Choi, H.J. Magnetorheology: materials and application. *Soft. Matter.*, **2010**, *6*(21), 5246–5253.
82. Kim, Y., Langari, R., Hurlebaus, S. Semiactive nonlinear control of a building with a magnetorheological damper system. *Mech. Syst. Signal Process.*, **2009**, *23*(2), 300–315.

CHAPTER 2

CLASSIFICATION OF SMART MATERIALS

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ABSTRACT

A set of materials that show the tendency to respond to modification in the surrounding environment by simply changing one or more of its properties are categorized as smart materials. For instance, piezoelectric materials result in the generation of electric fields in response to applied deformation, which makes them potent candidates for ultrasonic wave generation and sensors for detecting shape modification. Owing to the adaptive nature of these materials, they find several applications in the field of optoelectronic devices, sensors, actuators, and so on. Since we have a vast range of smart materials categorizing them would benefit inappropriate selection as per the need of the application. Therefore, these materials can be categorized into three classes: Type I, Type II, and Type III, reliant upon the responding element present in them. Type I materials are known as passive materials where an integrated sensor is incorporated into the structure for determining the stimuli and retorting to it. Fiber-optic-based sensors fall under this category. Type II materials are those materials that have an inbuilt nervous system and an actuator that shows the ability to change their structure or any other property under the influence of applied electric, magnetic, or thermal modifications.

2.1 INTRODUCTION

In the last few decades, smart materials have attracted considerable research interest for the progress of futuristic and sustainable devices owing to their ability to replicate human biological system [1–5]. These adaptive materials respond to the detected changes of heat, stress, electric and magnetic fields, or exposure to radiation in environment by modifying one or more of its properties like dimensions, viscosity, and vibrations [6]. More specifically, smart materials are nonbiological systems that are embedded/attached with the components which respond in predefined manner and hence possess the tendency to show functionality similar to biological systems. For instance, components like sensors present in them acts as the nervous system as they are responsible for data collection for sensing and forwarding the same to control and command unit, actuators behave like muscles as react toward the sensed data by activating the device where performance of real-time processors resembles the functioning of brain as it controls the whole process by computing the recorded data and taking necessary actions.

Features like self-adaptability, multifunctionality, sensibility, and intelligence to respond associated with these materials make these devices highly suitable for applications in aeronautics, structure manufacturing, sensor development, and actuation devices [7–13]. In addition, improvements in the present state of technology such as mechanical properties, destruction acceptance, sustainable manufacturing, and technological behavior are needed to make them appropriate for future challenges. Due to the wide range of uses of these materials and requirement for further development, categorization of various characteristics and properties are highly required as it will assist in material selection and essential modifications as per the specific need of applications. The prime motive of this chapter is to identify the criteria that can be used for the classification of existing smart materials, recent developments in the area, and their prominent applications.

2.2 CRITERIA FOR CLASSIFICATION OF SMART MATERIALS

The presence of inbuilt components, that is, sensors, actuators, and their regulator mechanism make the smart systems to respond actively to external stimuli in small span of time as well as in a predefined manner. In addition to it, they regain their original properties after the removal of stimuli. Based upon the type of components existent in the structure, smart materials can be categorized in the following three categories:

1. *Type I* materials are inherited with a nervous system and actuator control, enabling them to alter their behavior in response to various stimuli such as heat, light, humidity, mechanical stress, and electric and magnetic fields. The observed changes in the properties can be reversible and the materials can be designed to perform specific functions such as actuation and control. Due to their ability to show a change in physical property, these materials are also known as reactive or active smart structures.
2. *Type II* materials, also known as sensory structures, sense the structural as well as environmental modifications without requiring an external energy source or control system due to the presence of microsensor in their structure. These materials do not convert any energy in reaction to the changes they detect, and are therefore known as passive materials.
3. *Type III* or intelligent materials are a combination of Type I and Type II materials as they contain both the sensors and actuators where both the components work in sync to identify and respond to the external stimuli. More specifically, these structures have the ability to sense changes in their environment, process that information, and respond in a predetermined manner.

Figure 2.1 displays different set of smart materials available. Also the technology used by them for responding to the stimuli is indicated. Detailed discussion of their working as well as features are given in the upcoming sections.

2.3 ACTUATING SYSTEMS

An actuator is a device that accepts a signal from a control system and converts it into a physical action. Hence, actuators are crucial part of systems where organized and reactive behavior is required. For instance, a motor can receive a voltage signal and convert it into rotational motion, allowing it to control the position or speed of a mechanical system. Actuators are furnished either by bonding on the material surface or incorporated inside the bulk matrix. Several research works have been conducted in the past decade to find an appropriated actuator for industry as well as military applications, however, rigorous research in this direction is still required. Choice of actuating component to be used in a material depends on numerous aspects such as type of needed actuation, type of driving energy, and environmental factors.

In addition, behavior of actuator including energy losses, type of response generated, and time taken to respond are also considered. Depending upon the aforementioned factors, various types of actuating systems are available and are discussed in the following sections.

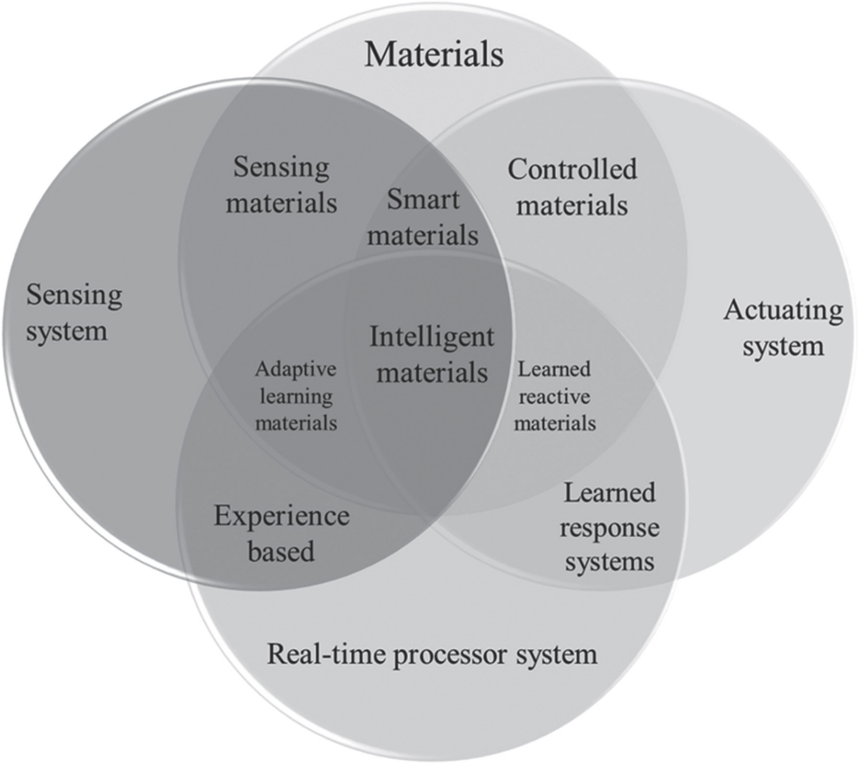
Materials
Sensing materials
Smart materials
Controlled materials
Sensing system
Actuating system
Intelligent materials
Adaptive learning materials
Learned reactive materials
Experience based
Learned response systems
Real-time processor system

FIGURE 2.1 Categorization of smart systems and their technologies. ⏎

2.3.1 THERMO-RESPONSIVE MATERIALS

Thermo-responsive materials, commonly known as shape memory alloys (SMA), exhibit an extraordinary feature of changing its crystalline structure in reply to modification in temperature or applied stress [14]. In these materials, there are at least two elementary phases: (1) austenite and (2) martensite, which undergo transformation during the distortion and recovery process. The face-centered cubic crystal structure known as austenite is stable at elevated temperatures and was discovered by Sir William Chandler

Roberts-Austen in 1890 [15]. Martensite, on the other hand, is a body-centered tetragonal crystal structure that is formed when certain alloys are cooled rapidly from high temperatures. Martensite is entitled after Adolf Martens, a German metallurgist who first described this structure in 1890 [16]. In thermo-responsive materials, the martensitic phase is the deformed shape of the material, while the austenitic phase is the original shape.

When an SMA is cooled below a specific temperature, called the martensitic transformation temperature, it experiences a phase conversion from its austenitic phase to its martensitic phase. In this martensitic phase, the material can be effortlessly distorted and takes on a new shape [17]. In contrast, when the same materials is heated beyond its transformation temperature, the reverse phase transformation occurs, and the material relapses to its previous austenitic phase. The temperature at which this transformation takes place is known as the austenitic transformation temperature. This phenomenon of regaining its original shape is acknowledged as shape memory effect.

SMAs may also experience a stress-induced transformation, where the application of stress can trigger a phase transformation leading to a change in shape. This stress-induced transformation occurs when the stress applied to the material is superior to a critical stress threshold, called as the transformation stress. After the removal of stress, the SMA returns to its original form through the reverse transformation process [18, 19].

The phenomenon of shape recovery was first observed in 1932 by Swedish metallurgist Arne Olander while studying the properties of gold–cadmium alloys [20]. However, it was not until the 1960s that the effect was fully understood and commercialized. After extensive research in the field, a similar phenomenon was observed in another set of materials. Among those materials, NiTi (53–57 wt.% Ni) and the Nitinol alloy system showed this phenomenon significantly such that it can be used for various commercial applications [21–23]. The shape memory effect has been extensively studied and researched, leading to the finding of many new SMA and selected of them are listed in Table 2.1.

It has been reported that several parameters like choice of composition for SMAs [32–39], postpreparation treatments including application of heat and mechanical treatments [40–48], cooling technique [49–52], modified surface [53–57], and choice of preparation methods [58–60] determine the behavior of developed SMA. Furthermore, the properties are nonlinearly dependent on the mentioned parameters, necessitating extensive research in this area.

Depending upon the external conditions, SMAs exhibit several types of mechanical behaviors (shown in Figure 2.2), including: thermoelasticity,

TABLE 2.1 Recently Reported Shape Memory Allows Along With Their Characteristics Such As Martensite Finish Temperature (*M_f*), Martensite Start Temperature (*M_s*), Austenite Start Temperature (*A_s*) and Austenite Finish Temperature (*A_f*)

Alloy	Composition	M_f (°C)	M_s (°C)	A_f (°C)	A_s (°C)	References
Fe–Mn–Si	Fe-17Mn-5Si-10Cr-4Ni-1 (mass%)	−90	−75	110	85	[24]
Fe–Mn–Si	Fe-17Mn-5Si-10Cr-4Ni-1 (mass%)	−64	−60	162	103	[25]
Cu–Ni–Mn	Cu-11.6Al-3.2Ni-2.7Mn (wt.%)	–	274	–	191	[26]
Cu–Al–Ni	Cu-14 wt.% Al-4.2 wt.% Ni	41	53	66.5	48	[27]
Cu–Zn–Al	Cu-21.5 wt.% Zn-5.85 wt.% Al	57	69	81	70	[27]
Ni–Ti–Cu	Ni-32 wt.% Ti-47 wt.% Cu-21 wt.%	31.7	–	41.2	–	[28]
Ni–Pd–Ti–Hf	Ni-35 wt.% Pd-15 wt.% Ti-30 wt.% Hf-20 wt.%	470	525	686	537	[29]
Ni–Ti–Hf	Ni-50.3 Ti-29.7 Hf-20 at.%	129	143	172	159	[30]
Cu–Al–Ni–Ta	79% wt Cu-13% wt Al-4% wt Ni-4% wt Ta	104.4–141.1	149.8–2185.8	188.4–293.6	139.1–187.6	[31]

superelasticity, pseudoplasticity, damping capacity, and actuation. Thermoelasticity is a term used to describe the reversible deformation of SMA due to thermal cycling between two temperatures, one above and one below the phase conversion temperature of the material. Based upon the steps followed to recover the original shape, these are categorized as one- and two-way SMA. During this cyclic process, temperature loss takes place which is called as hysteresis. Jani et al. [61] has explained the process in details. Materials showing one-way effect find potential applications in actuators.

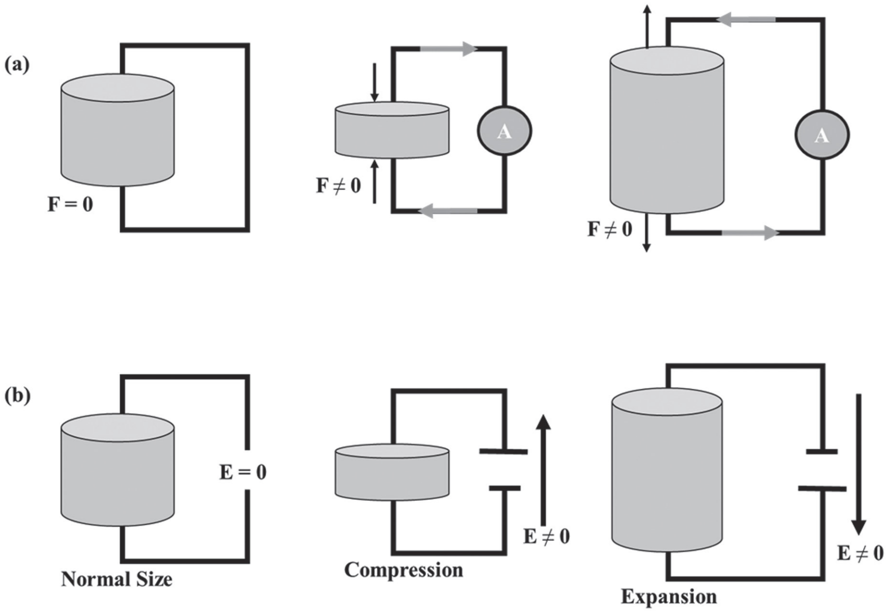

FIGURE 2.2 Systematic representation of (a) direct and (b) converse piezoelectric effect where *F* represents the applied force and *E* represents the applied electric field. ⏎

Another property is superelasticity, also known as pseudoelasticity, is a nonlinear mechanical property where the material can undergo great reversible distortions without suffering permanent plastic distortion or failure. It is possible to obtain almost reversible deformations up to strains of 10^{-1} or higher, with a very small effective modulus compared to the elastic moduli of the parent material because of reversible phase change that occurs between the austenitic and martensitic phases of the material under certain conditions [62, 63]. When the SMA is in the austenitic phase, a high modulus of elasticity is exhibited by the material and it behaves like a typical elastic material. However, when the SMA is subjected to stress or strain above a certain threshold, it can transform to the martensitic phase, resulting in a significant decrease in modulus and the capability to experience large distortions without permanent distortion. After the stress or strain is removed, material transmute to the austenitic phase, resulting in almost complete shape recovery. The effective modulus of the material during this superelastic deformation is much lower than that of the parent material due to the reorientation of the martensitic variations that occurs during the transformation [64].

On the other hand, pseudoplasticity is the procedure of deformation that occurs in small steps till a very large strain is applied where the process becomes irreversible in nature even after the removal of residual strain. However, the initial shape can be retrieved by heating the material [65, 66]. Martensite demonstrates lower crystal symmetry than the austenite phase. The presence of polydomained microstructures in the martensite phase contributes to this characteristic, as they consist of physically similar domains oriented in different directions [67, 68]. More specifically, no stress is generated because of contact of polydomains due to their self-strain compatibility in the direction of plane boundaries. The change in domain ratio resulting from the displacement of boundary facilitates the formation of deformed martensite, leading to pseudoplasticity. The various structures achieved can be reverted back to their original state through material heating. Additionally, when the load applied is minimal, deformation occurs without hardening, allowing for the restoration of the initial stage upon stress removal.

In addition, damping capacity referred to as the capability to dissipate energy into internal energy when subjected to vibrational stress. In simpler terms, the material's ability to resist the transmission of mechanical energy is known as its capacity. Shape memory alloys (SMAs) undergo phase transformation, allowing them to recover significant amounts of strains [61, 69]. These alloys are effective at dissipating energy for strains greater than 10^{-5} units [70], with the amplitude of vibrations playing a crucial role. However, the material's energy dissipation capacity is contingent on its composition and microstructures.

Shape memory alloy fibers (SMAF) implanted in composite matrix acts as an actuator that can be used to monitor static as well as dynamic behavior of the material. Active property tuning (APT) and active strain energy tuning (ASET) are the two monitoring procedures on which shape memory fiber actuators work [71, 72]. Shame memory effect and large Young's modulus during phase transformation are the two prime features that provide the material with exceptional strain recovering ability and restoring force. Through APT, incorporated SMAF are actuated by the application of electric current that results in rise of temperature. Once the temperature rises beyond austenitic transformation temperature, the Young's modulus of materials is increased in a predefined manner [73]. Whereas, in ASET, it has been observed that polymer systems incorporate already lengthened fibers, which become inelastic [73]. When an electric field is applied, the system heats up, causing the embedded fibers to contract and recover their original shape, leading to an increase in stress recovery.

2.3.2 PIEZOELECTRIC MATERIALS

Piezoelectricity is a phenomenon through which materials produce an electric charge when they are exposed to mechanical pressure [74]. This phenomenon was first discovered in 1880 by Pierre Curie and Jacques Curie [75, 76]. It was originally thought that mechanical deformation played a significant role in generating electricity. However, further exploration into thermodynamic principles revealed that this phenomenon also exhibits reversibility. In other words, the application of an electric field can cause changes in the dimensions of a material, known as the reverse piezoelectric effect.

Piezoelectric materials possess unique crystal structure that facilitate them to produce an electric charge in reaction to a compression/expansion. Subjection of material to mechanical stress results in the displacement of atoms in the crystal lattice from their equilibrium positions, causing a separation of positive and negative charges. Eventually, this polarization of charges leads to the generation of an electric field that can be measured as a current across the material. The direction of the flow of current depends on the direction of the applied force. Figure 2.2a displays the generation of current through piezoelectric effect. Moreover, if the same material is exposed to exterior electric field, modification in the dimensions of it can be observed due to discharge of energy in form mechanical stress (Figure 2.2b) [77]. Electric current can also be generated in contact electricity and pyroelectricity when friction and heat are produced in the material [78].

The degree of polarization or the field generated is proportional to smeared mechanical stress whereas the moduli of piezoelectricity is related to a third rank tensor (d_{ijk}) [79]. Same tensor also determines the produced strain in response to provided eternal field in converse piezoelectric effect.

By embedding/depositing the piezoelectric material in/on a composite material in an appropriate form, actuating properties can be achieved.

Initially, the subdomains of crystals in the film are oriented along with the thickness of the material by the application of strong field of around 2 kV mm^{-1} known as poling. This exercise allows the piezoelectric material to develop along the field and contract normally. These subdomains are stable at temperature lower than Curie temperature. After the consequent exposure of the material to electric field, poled domains begin to grow in its direction and results in normal contraction strain. Whereas, solicitation of reverse field leads to reduction in thickness till an opposite field magnitude is not achieved. After the achievement of negative field, direction of poling changes and hence thickness begins to increase gain. A significant quantity of piezoelectric polycrystalline ceramics and polymers have been documented.

2.3.3 ELECTROSTRICTIVE MATERIALS

Like piezoelectric materials, electrostrictive materials exhibit only an increase in shape or size when subjected to an electric field, and the size increases even with the change in polarity of the applied field [80, 81]. The alteration occurs due to the reorganization of charges within the material, leading to a redistribution of internal stresses and strains. Nonetheless, the electrostrictive effect is significantly less pronounced compared to the piezoelectric effect. Furthermore, piezoelectric actuators exhibit nonlinearity and heightened reactivity, particularly when exposed to large alternating fields, which is considered a primary disadvantage of the material [82, 83]. Conversely, electrostrictive materials do not display such behavior [80, 84]. Their magnitude varies quadratically as a function of applied field. Some common examples of electrostrictive materials include ceramics such as lead magnesium niobate (PMN) and lead zirconate titanate (PZT), as well as certain polymers and composites which shows zero production of piezoelectricity with no hysteretic behavior and are nonlinear [84, 85]. Their low hysteresis makes them suitable for open-loop shape control applications. Unlike piezoelectric materials, electrostrictive materials do not need to undergo poling to achieve their desired properties. Despite their potential advantages, however, there has been relatively little work on the use of electrostrictive materials in smart composites. This may be due in part to the fact that the strain effect in these materials is nonlinear and decreases with temperature, which can limit their usefulness in certain applications.

2.3.4 MAGNETOSTRICTIVE MATERIAL

Magnetostrictive materials are a class of materials that undergo a modification in shape or size in reaction to applied magnetic field. This phenomenon is known as magnetostriction and is caused by the reorientation of the magnetic domains within the ferromagnetic material. The change in shape or size is typically small, but it is highly responsive to changes in the magnetic field, making magnetostrictive materials useful for a variety of actuating applications [86].

After the subjecting a magnetostrictive material to magnetic field, the magnetic subdomains present in it begin to arrange themselves in the direction of applied field. This causes a change in the internal stress distribution within the material, which results in an alteration in the material's dimensions. The direction and magnitude of this change depend on the orientation and strength of the magnetic field and the material's magnetostrictive coefficient [86]. The whole procedure is depicted in Figure 2.3.

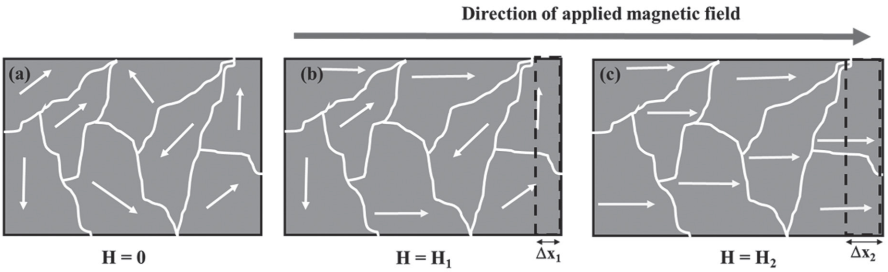

FIGURE 2.3 Illustration of magnetostriction effect, that is, modification in shape of the material after the subject of magnetic field. (a) Represents the magnetic domains in absence of magnetic field and its direction is represented with arrow. Whereas, with the use of magnetic field the magnetic subdomains begins to align in the direction of magnetic field due to the development of the strain. In (b), the length increases by Δx_1, and in (c), the length increases by Δx_2 with the application of field of strength H_1 and H_2, respectively, where $H_2 > H_1$. ⏎

In these materials, a magnetic field can be produced through a cyclic process. When subjected to a magnetic field, magnetostrictive materials experience a mechanical stress in response to a change in shape. This generated stress can then be used to induce a magnetic field through the Villari effect [86]. The production of a magnetic field is illustrated in Figure 2.4.

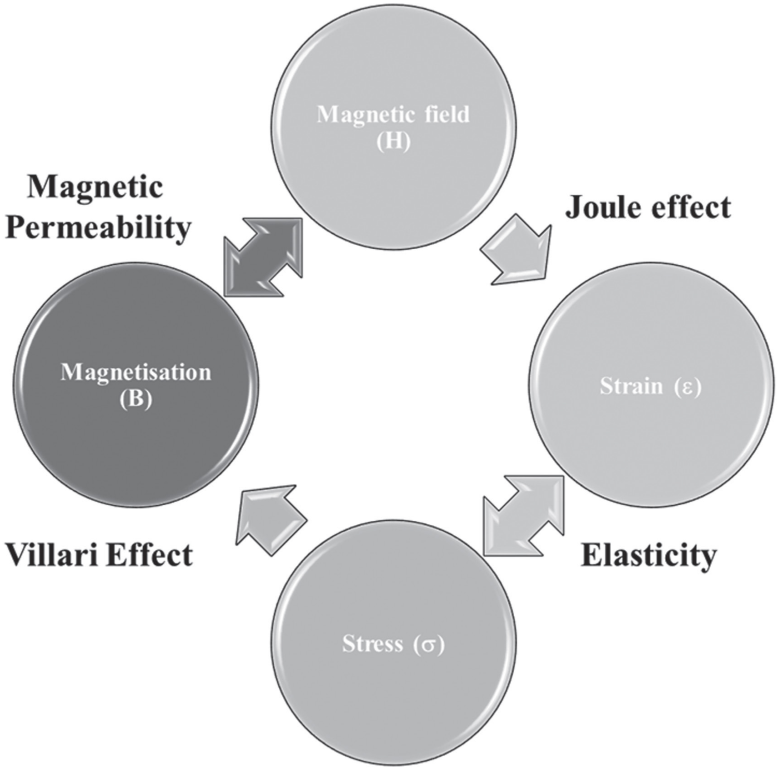
Magnetic field (H)
Joule effect
Strain (ε)
Elasticity
Stress (σ)
Villari Effect
Magnetisation (B)
Magnetic Permeability

FIGURE 2.4 Schematic representation of cyclic production of magnetic field by magnetostriction materials. ⏎

2.3.5 pH SENSITIVE MATERIALS

pH-sensitive smart materials are an important member of family of smart materials that can show alteration in physical/chemical properties in reaction to modifications in the pH of their surrounding conditions [87]. These materials can be classified into two main groups: acidic and basic materials. Acidic materials have functional groups that can provide a proton in response to an increase in pH, while basic materials have functional groups that can receive a proton in response to a decrease in pH [88]. These materials are often used in sensing, drug delivery, and biomedical applications, as well as in environmental monitoring [89].

One common type of pH-sensitive smart material is a hydrogel. Hydrogels are cross-linked polymer networks that can swell/shrink in reaction to variation in pH. When the pH of the environment changes, the functional groups within the hydrogel either donate or accept protons, causing the polymer chains to either expand or contract. This change in volume can be applied to regulate the discharge of drugs or other molecules that are encapsulated within the hydrogel [90].

Another type of pH-sensitive smart material is a pH indicator. pH indicators are compounds that change color in response to changes in pH [91]. These materials are often used in pH sensing applications, such as in pH test strips or in environmental monitoring. For instance, hydrochromic materials are used in bandages to identify the pH modification in skin while convalescing from any injury [92].

2.3.6 ELECTRORHEOLOGICAL FLUIDS AND MAGNETORHEOLOGICAL FLUIDS

Fluids are classified as either Newtonian or non-Newtonian based on their viscosity behavior. Newtonian fluids demonstrate a direct correlation between shear stress and shear rate, indicating that their viscosity remains constant regardless of the applied shear rate. In contrast, non-Newtonian fluids do not follow this linear relationship and can adjust their viscosity depending on the shear rate or shear stress they are subjected to. The viscosity of non-Newtonian fluids can be altered by factors such as shear rate, temperature, pressure, and composition. They can display behaviors such as shear-thinning (decreasing viscosity with increasing shear rate), shear-thickening (increasing viscosity with increasing shear rate), and viscoelasticity (exhibiting both liquid and solid-like properties).

Electrorheological fluids are non-Newtonian fluids that finds potential applications in fluid-based actuating devices as they exhibit a significant change in their rheological properties, particularly viscosity, when an electric field is subjected. They are colloidal suspensions consisting of electrically polarizable particles distributed in a liquid medium, typically an insulating oil [93]. On the application of electric field, the electrically polarizable particles in the fluid align themselves in chains or structures, forming a network-like structure. This network hinders the flow of the fluid, resulting in a significant increase in viscosity. Also, after the removal of electric field, the particles disperse randomly, and the fluid returns to its low-viscosity state. The electrorheological outcome can be controlled by adjusting the strength of applied electric field, allowing for precise modulation of the fluid's rheological properties. The response time of electrorheological fluids is typically in the millisecond range, making them potent applicant for sensing applications [94].

Similar to electrorheological fluids, magnetorheological fluids are also colloidal suspensions consisting of magnetizable particles dispersed in a carrier fluid, typically a base oil, and can undergo reversible changes in their rheological properties in the existence of a magnetic field [95, 96]. These materials are highly suitable for applications that require rapid and reversible changes in viscosity. The behavior of MR fluids is controlled by the application of an external magnetic field. When no magnetic field is present, the suspended particles are arbitrarily dispersed within the fluid, allowing it to flow freely with low viscosity. However, after the application of magnetic field, the particles arrange themselves along the magnetic field lines, forming chains or clusters. This alignment causes the fluid to undergo a rapid and significant growth in viscosity, often by some orders of magnitude. In addition, the rheological response of MR fluids can be adjusted by changing the magnitude of the magnetic field. The viscosity change occurs almost instantaneously with the application or removal of the magnetic field, allowing for precise and rapid control of the fluid's behavior [97, 98].

2.4 SENSORY SYSTEMS

With the help of a sensor, one can record a physical quantity and transform it into an electric signal which can be processed by a control system. For instance, a temperature sensor can sense alteration in temperature and change them into a voltage signal that can be read other electronic device. Embedment of a sensor into composite material can facilitate to interrogate the internal modifications in the material as a response to environmental changes. The sensors that can be used for this purpose are generally based on fiber optics as they offer promising application due to their fabrication compatibility and ability to sustain under required magnitude of strain. Apart from this, sensors based on piezoelectricity are also used. Based upon the working mechanism of incorporated sensor, sensor systems can be categorized in following categories.

2.4.1 FIBER-OPTIC SENSORS

Optical fibers are thin threads generally made up of glass that are used to communicate digital information, such as data, audio, or video signals, over long distances by transforming electrical signals into light and sending them through the fiber *via* the process known as total internal reflection. The fiber is made up of a core, which is the central region where the light travels, and a cladding layer, which is an outer layer that surrounds the core and has a lower refractive index than the core. Both core and clad are usually prepared from silica where either core or clad is doped to increase or decrease the refractive index, respectively, in order to satisfy the condition of total internal reflection. When light is introduced into the core of the fiber at one end, it is reflected back and forth between the core and the cladding layer due to the difference in refractive index, and it continues to travel along the length of the fiber without significant attenuation or loss of signal strength.

The light can be transmitted using either single-mode fibers, which have a small core (having diameter around 10 μm) that allows for a single light ray to travel along the fiber, or multimode fibers, which have a larger core diameter ranging from 50 μm to more than 100 μm that allows for multiple light rays to travel along the fiber simultaneously. The choice of fiber depends on the specific application and the distance over which the light needs to be transmitted.

Optical fibers are encased in a protective layer, commonly composed of polymer materials like acrylate or polyimide. This coating safeguards the fragile fibers from potential harm caused by moisture, chemicals, and external elements. Additionally, (1) the protective layer acts as lubrication, facilitating easier handling during installation and maintenance, thereby lowering the risk of damage or breakage, (2) it provides a buffer between the fiber and any surrounding materials, helping to prevent light from leaking out of the fiber, and (3) it can be colored to help identify different fibers or to indicate specific functions or uses.

Optical fiber-based sensors are attracting significant research interest as they can be developed to identify all the possible parameters related to physical, chemical and biological properties [99–103]. Their compact size facilitates with easy incorporation into material and promotes continuous recording of observed structural changes right beginning form the process of fabrication throughout the lifespan providing benefits such as early detection of structural issues, increased safety and reliability, reduced downtime, and improved overall performance and longevity. Most, if not all, optical fibers are silica-based, providing compatibility with various materials and high strain tolerance. These sensors are known for their accurate data transmission, as the fiber's data is not affected by external electric or magnetic fields. This is especially attractive for applications within carbon fiber reinforced plastic components where electrically isolating sensor arrays from the reinforcing fibers present significant difficulties. Moreover, their light weight makes them potential applicants for several aeronautical applications [104, 105].

Selecting the appropriate coating is essential while designing optical fiber sensors because the coating material can affect the sensitivity, accuracy, and durability of the sensor [106, 107]. The coating material must be compatible with the sensing mechanism and the measurement environment to ensure that the sensor performs accurately and reliably over time. Additionally, the coating thickness and refractive index can affect the sensitivity of the sensor by altering the way light interacts with the sensing element [108, 109]. Therefore, selecting a coating material with the appropriate thickness and refractive index is important to optimize the sensor's performance. Furthermore, the coating material can affect the sensor's response time, linearity, operating temperature, and other performance characteristics. Therefore, selecting the appropriate coating material is crucial to ensure that the sensor meets the desired specifications for the specific application.

2.4.2 PIEZOELECTRIC SENSORS

Piezoelectric materials can also be utilized to measure various physical quantities, such as pressure, strain, and vibration. The construction of a piezoelectric sensor typically involves a piezoelectric material, such as quartz, ceramic, or certain polymers, sandwiched between two electrodes [110]. When the sensor is exposed to the physical quantity under measurement, it undergoes deformation, leading to the application of mechanical stress or pressure on the piezoelectric material. This stress results in the displacement of the atoms within the material, leading to the separation of charges and the production of an electric potential across the electrodes.

The construction of a piezoelectric sensor typically involves a piezoelectric material, such as quartz, ceramic, or certain polymers, sandwiched between two electrodes. Mostly, the electrodes are made up of polymers as their low density and hence facilitates with improved impedance matching. Severely, these are also made up of metal. Sandwiching between electrodes reduces the chance of breakage due to brittle nature of piezoelectric crystal and hence improves efficiency of the sensors [111–113]. When the sensor experiences the physical quantity it is measuring, it undergoes deformation, exerting mechanical stress or pressure on the piezoelectric material. This mechanical stress causes the material's atoms to shift, resulting in the separation of charges and the generation of an electric potential across the electrodes. This potential can be measured and converted into a corresponding electrical signal, which can be further processed, displayed, or transmitted for analysis or control purposes.

Piezoelectric sensors have several advantages that make them suitable for various applications. They offer high sensitivity, allowing for precise measurements in dynamic conditions. They have a wide frequency response, enabling the detection of rapid changes and vibrations [114, 115]. Piezoelectric sensors are also durable, compact, and can operate in harsh environments, including high temperatures and pressures.

These sensors find applications in multiple industries and fields. For example, in automotive engineering, they are used for measuring engine vibrations, tire pressure, and crash detection. In medical devices, piezoelectric sensors are utilized for ultrasound imaging, heartbeat monitoring, and drug delivery systems. They are also commonly employed in industrial manufacturing, aerospace, robotics, and civil engineering for monitoring structural integrity, material testing, and quality control.

2.5 INTELLIGENT SYSTEMS

Material comprising both sensors and actuators are termed as intelligent systems as the signal received by the sensor is processed by microprocessor-based controllers and activate the actuator to respond to it. The use of parallel processing with neural networks in real-time controllers is gaining attention in this field. Neural networks are composed of coatings of simple nonlinear components that have the ability to learn and make decisions collectively, similar to how biological systems function. They can handle adaptive learning, quick processing, and executive tasks. In the context of assessing the structural integrity of an aircraft, it would be necessary to have comparative reference values obtained from flying the aircraft and gathering tension and heat information from precarious areas. Neural networks with self-adaptive processing capabilities are well-suited to handle the large volumes of data that would be generated in such scenarios. Progress in developing neural network-based controllers for fully intelligent materials is still in its early stages, but significant advancements are expected in the near future.

2.6 CONCLUSIONS

Smart materials encompass a diverse range of materials with unique properties and functionalities. This chapter delves into the categorization of smart materials according to their fundamental mechanisms and capabilities. Examples include piezoelectric materials, SMAs, electroactive polymers, magnetorheological materials, thermoelectric materials, and photomechanical materials. Understanding these classifications is essential for researchers, engineers, and designers to choose appropriate material for specific application. Each class of smart materials offers distinct properties, making them suitable for specific tasks and environments. The field of smart materials continues to evolve, with ongoing research and development aimed at enhancing their properties and expanding their applications. Researchers in the field of science and engineering are continuously investigating innovative materials, experimenting with unique capabilities, and enhancing current smart materials to meet the increasing needs of diverse industries.

KEYWORDS

- **smart materials**
- **classification**
- **technologies**
- **mechanisms**
- **functionalities**

REFERENCES

1. Kök, M., Qader, I.N., Dağdelen, F., Aydoğdu, Y. Akıllı Malzemeler üzerine derleme: araştırmalar ve uygulamaları. *El-Cezeri Fen ve Mühendislik Derg.*, **2019**, *2019*, 755–788, https://doi.org/10.31202/ecjse.562177.
2. Zhang, Z., Demir, K.G., Gu, G.X. Developments in 4D-printing: a review on current smart materials, technologies, and applications. *Int. J. Smart Nano Mater.*, **2019**, *10*, 205–224, https://doi.org/10.1080/19475411.2019.1591541.
3. Yu, X., Cheng, H., Zhang, M., Zhao, Y., Qu, L., Shi, G. Graphene-based smart materials. *Nat. Rev. Mater.*, **2017**, *2*, 1–14, https://doi.org/10.1038/natrevmats.2017.46.
4. Mendes, C.-Felipe, Oliveira, J., Etxebarria, I., Vilas-Vilela, J.L., Lanceros-Mendez, S. State-of-the-art and future challenges of UV curable polymer-based smart materials for printing technologies. *Adv. Mater. Technol.*, **2019**, *4*, 1–16, https://doi.org/10.1002/admt.201800618.
5. de Oliveira, R.F. change the ChangetheRest, White, O., Kerlavage, A.R., Clayton, R.A., Sutton, G.G., Fleischmann, R.D., Ketchum, K.A., Klenk, H.P., Gill, S., Dougherty,

B.A., Nelson, K., Quackenbush, J., Zhou, L., Kirkness, E.F., Peterson, S., Loftus, B., Richardson, D., Dodson, R., Khalak, H.G., Glodek, A., Mckenney, K., Fitzegerald, L.M., Lee, N., Adams, M.D., Hickey, E.K., Berg, D.E., Gocayne, J.D., Utterback, T.R., Peterson, J.D., Kelley, J.M., Cotton, M.D., Weidman, J.M., Fujii, C., Bowman, C., Watthey, L., Wallin, E., Hayes, W.S., Borodovsky, M., Karpk, P.D., Smith, H.O., Fraser, C.M., Venter,J.C. Enhanced Reader.pdf. *Nature*, **2018**, *388*, 539–547.

6. Cao, W., Cudney, H.H., Waser, R. Smart materials and structures. *Proc. Natl. Acad. Sci. U. S. A.*, **1999**, *96*, 8330–8331, https://doi.org/10.1073/pnas.96.15.8330.
7. Straub, F.K., King, R.J. Application of smart materials to control of a helicopter rotor. In *Proceedings of SPIE 2721, Smart Structures and Materials 1996: Industrial and Commercial Applications of Smart Structures Technologies*, 1 May 1996, pp. 66–77, https://doi.org/10.1117/12.239159.
8. Sponchioni, M., Capasso Palmiero, U., Moscatelli, D. Thermo-responsive polymers: applications of smart materials in drug delivery and tissue engineering. *Mater. Sci. Eng. C.*, **2019**, *102*, 589–605, https://doi.org/10.1016/j.msec.2019.04.069.
9. Bogue, R. Smart materials: a review of capabilities and applications. *Assem. Autom.*, **2014**, *34*, 16–22, https://doi.org/10.1108/AA-10-2013-094.
10. Cruz, M., Kyung, K.U., Shea, H., Bose, H., Graz, I. Applications of smart materials to haptics. *IEEE Trans. Haptics.*, **2018**, *11*, 2–4, https://doi.org/10.1109/TOH.2018.2809058.
11. R. M-, William, B. Patent: Monolithic piezoelectric sensor (MPS) for sensing chemical, biochemical and physical measurands, 2000.
12. Examiner, P., Lefkowitz, E., Vanderhye, P.C. (12) United States Patent, 2, 2006.
13. Wieszczycka, K., Staszak, K., Woźniak-Budych, M.J., Litowczenko, J., Maciejewska, B.M., Jurga, S. Surface functionalization—the way for advanced applications of smart materials. *Coord. Chem. Rev.*, **2021**, *436*, https://doi.org/10.1016/j.ccr.2021.213846.
14. Otsuka, K., Ren, X. Recent developments in the research of shape memory alloys. *Intermetallics*, **1999**, *7*, 511–528, https://doi.org/10.1016/S0966-9795(98)00070-3.
15. Kayser, F.X., Patterson, J.W. Sir William Chandler Roberts-Austen—his role in the development of binary diagrams and modern physical metallurgy. *J. Phase Equilib.*, **1998**, *19*, 11–18, https://doi.org/10.1007/bf02904718.
16. Kumar, S., Shahi, A.S. Effect of heat input on the microstructure and mechanical properties of gas tungsten arc welded AISI 304 stainless steel joints. *Mater. Des.*, **2011**, *32*, 3617–3623, https://doi.org/10.1016/j.matdes.2011.02.017.
17. Lagoudas, D.C. Shape memory alloys: modeling and engineering applications. 2008. https://link.springer.com/book/10.1007/978-0-387-47685-8.
18. Krulevitch, P., Lee, A.P., Ramsey, P.B., Trevino, J.C., Hamilton, J., Northrup, M.A. Thin film shape memory alloy microactuators. *J. Microelectromech. Syst.*, **1996**, *5*, 270–282, https://doi.org/10.1109/84.546407.
19. Gu, H., Bumke, L., Chluba, C., Quandt, E., James, R.D. Phase engineering and supercompatibility of shape memory alloys. *Mater. Today.*, **2018**, *21*, 265–277, https://doi.org/10.1016/j.mattod.2017.10.002.
20. Alloys, S.C. Cadmium-gold alloys solid. *J. Am. Chem. Soc.*, **1932**, *337*.
21. Markopoulos, A.P., Pressas, I.S., Manolakos, D.E. A review on the machining of nickel-titanium shape memory alloys. *Rev. Adv. Mater. Sci.*, **2015**, *42*,28–35.
22. Buehler, W.j., Wang, F. E. A summary of recent research on the nitinol alloys and their potential application in ocean engineering. *Ocean Eng*. **1968**, *1*, 105–120.

23. Kawarada, Y., Aimi, A., Santos, A., Nakata, G., Takeuchi, I. Abnormal grain growth of 68Cu–16Al–16Zn alloys for elastocaloric cooling via cyclical heat treatments. *J. Phys.* **2023**, *5*, 024012..
24. Dong, Z., Klotz, U.E., Leinenbach, C., Bergamini, A., Czaderski, C., Motavalli, M. A novel Fe-Mn-Si shape memory alloy with improved shape recovery properties by VC precipitation. *Adv. Eng. Mater.*, **2009**, *11*, 40–44, https://doi.org/10.1002/adem.200800312.
25. Gao, Z.Y., Yang, S., Zhang, H.J., Dong, G.F., Cai, W. Effect of aging on phase transformation, thermoelastic and fracture behavior of Mn 53 Ni 25 Ga 22 ferromagnetic shape memory alloy. *Mater. Sci. Eng.*, **2014**, *594*, 1–6.
26. Rodríguez-Aseguinolaza, J., Ruiz-Larrea, I., Nó, M.L., López-Echarri, A., Bocanegra, E.H., San Juan, J. Thermal history effects of Cu-Al-Ni shape memory alloys powder particles compared with single crystals behaviour. *Intermetallics.*, **2010**, *18*, 2183–2190, https://doi.org/10.1016/j.intermet.2010.07.002.
27. Wang, Z.G., Zu, X.T., Yu, H.J., He, X., Peng, C., Huo, Y. Temperature memory effect in CuAlNi single crystalline and CuZnAl polycrystalline shape memory alloys. *Thermochim. Acta.*, **2006**, *448*, 69–72, https://doi.org/10.1016/j.tca.2006.05.021.
28. Trehern, W., Ortiz-Ayala, R., Atli, K.C., Arroyave, R., Karaman, I. Data-driven shape memory alloy discovery using Artificial Intelligence Materials Selection (AIMS) framework. *Acta Mater.*, **2022**, *228*, 117751.
29. Canadinc, D., Trehern, W., Ma, J., Karaman, I., Sun, F., Chaudhry, Z. Ultra-high temperature multi-component shape memory alloys. *Scr. Mater.*, **2019**, *158*, 83–87, https://doi.org/10.1016/j.scriptamat.2018.08.019.
30. Hayrettin, C., Karakoc, O., Karaman, I., Mabe, J.H., Santamarta, R., Pons, J. Two way shape memory effect in NiTiHf high temperature shape memory alloy tubes. *Acta Mater.*, **2019**, *163*, 1–13, https://doi.org/10.1016/j.actamat.2018.09.058.
31. Kök, M., Qader, I.N., Mohammed, S.S., Oner, E., Dağdelen, F., Aydogdu, Y. Thermal stability and some thermodynamics analysis of heat treated quaternary CuAlNiTa shape memory alloy. *Mater. Res. Express.*, **2019**, *7*, https://doi.org/10.1088/2053-1591/ab5bef.
32. Ibrahim, M.K., Hamzah, E., Saud, S.N., Nazim, E.M., Iqbal, N., Bahador, A. Effect of Sn additions on the microstructure, mechanical properties, corrosion and bioactivity behaviour of biomedical Ti-Ta shape memory alloys effect of sn additions on the microstructure, mechanical properties, corrosion and bioactivity behaviour O. *J. Therm. Anal. Calorim.*, **2018**, https://doi.org/10.1007/s10973-017-6636-2.
33. Mediha, K. The effect of addition of various elements on properties of NiTi-based shape memory alloys for biomedical application. **2017**, *132*, 185, https://doi.org/10.1140/epjp/i2017-11461-5.
34. Alloy, S.M. Ti 50 Ni 47 Fe 3 shape memory alloy. 2023.
35. Vrsalovi, L., Kosec, B. Applied surface science advances electrochemical behaviour of CuAlMn alloy in the presence of chloride and sulphate ions Alě. **2023**, *13*, https://doi.org/10.1016/j.apsadv.2023.100380.
36. Balci, E., Dagdelen, F. Effects of substituting Nb with V on thermal analysis and biocompatibility assessment of quaternary NiTiNbV. *Eur. Phys. J. Plus.*, **2021**, *123*, https://doi.org/10.1140/epjp/s13360-021-01149-w.
37. Ko, M. Examination of phase changes in the CuAl high-temperature shape memory alloy with the addition of a third element. **2018**, *133*, 845–850., https://doi.org/10.1007/s10973-018-7176-0.

38. Ibrahim, M.K., Hamzah, E., Saud, S.N. Microstructure, phase transformation, mechanical behavior, bio-corrosion and antibacterial properties. *J. Mater. Eng. Perform*. **2019**, *28*, 382–393. https://doi.org/10.1007/s11665-018-3776-x
39. Biruke, F., Peng, B., Oliveira, J.P., Shen, J., Ao, S., Li, H., Chen, L., Tan, C., Song, X., Zhou, N., Zeng, Z. Materials & design role of Pd interlayer on NiTi to Ti6Al4V laser welded joints: microstructural evolution and strengthening mechanisms. *Mater. Des.*, **2023**, *228*, 111845, https://doi.org/10.1016/j.matdes.2023.111845.
40. Qader, I.N., Kök, M., Dağdelen, F., Phys. B, Cond. Matter, **2018**, *553*, 1–5. https://doi.org/10.1016/j.physb.2018.10.021.
41. Dagdelen, F., Qader, I.N. Influence of Ni addition and heat treatment on phase transformation Influence of Ni addition and heat treatment on phase transformation temperatures and microstructures of a ternary CuAlCr alloy. 2019, https://doi.org/10.1140/epjp/i2019-12479-3.
42. Milosavljevic, D., Bassani, P., Cinquemani, S., Lecis, N. Effects of thermomechanical treatments on Cu–Al–Mn shape memory alloys. *Mater. Chem. Phys.*, **2023**, *302*, 127756, https://doi.org/https://doi.org/10.1016/j.matchemphys.2023.127756.
43. Kök, M., Aydogdu, Y. Thermochimica acta effect of heat treatment on the physical properties of Ni–Mn–Ga alloy. *Thermochim. Acta.*, **2012**, *548*, 51–55, https://doi.org/10.1016/j.tca.2012.08.030.
44. Luo, Q., Wen, H., Bu, D., Peng, H., Wen, Y. Correlation between shape memory effect and density of annealing twin boundary in an FeMnSiCrNi alloy during special heat treatments with different parameters. *Mater. Sci. Eng. A.*, **2022**, *859*, 144213, https://doi.org/https://doi.org/10.1016/j.msea.2022.144213.
45. Li, B., Wang, B., Wang, L., Oliveira, J.P., Cui, R., Wang, Y., Zhu, G., Yu, J., Su, Y. Effect of post-heat treatments on the microstructure, martensitic transformation and functional performance of EBF3-fabricated NiTi shape memory alloy. *Mater. Sci. Eng. A.*, **2023**, *871*, 144897, https://doi.org/https://doi.org/10.1016/j.msea.2023.144897.
46. Yang, C.H., Lin, H.C., Lin, K.M., Tsai, H.K. Effects of thermo-mechanical treatment on a Fe–30Mn–6Si shape memory alloy. **2008**, *497*, 445–450, https://doi.org/10.1016/j.msea.2008.07.057.
47. Qian, S.U.N., Bo, C.A.O., Takeshi, I., Tao, S.U.O. Effect of impact deformation on shape recovery behavior in Fe-Mn-Si shape memory alloy under shape memory training process with cyclic thermo-mechanical loading. **2021**, *64*, 1389–1400.
48. Yong, L., Luo, Q., Peng, H., Yan, J., Xu, B., Wen, Y. Materials characterization dependence of shape memory effect on austenitic grain sizes in thermo- mechanical treated Fe-Mn-Si-Cr-Ni shape memory alloys. *Mater. Charact.*, **2020**, *169*, 110650, https://doi.org/10.1016/j.matchar.2020.110650.
49. Saud, S.N., Hamzah, E., Abubakar, T., et al. Structure–property relationship of Cu-Al-Ni-Fe shape memory alloys in different quenching media structure-property relationship of Cu-Al-Ni-Fe shape memory alloys in different quenching media. *J. Materi. Eng. Perform.* **2014**, *23*, 255–261, https://doi.org/10.1007/s11665-013-0759-9.
50. Saud, S.N., Hamzah, E., Abubakar, T., Farahany, S. Effects of quenching media on phase transformation characteristics and hardness of Cu-Al-Ni-Co shape memory alloys. 2015, https://doi.org/10.1007/s11665-015-1436-y.
51. Alloy, C.S.M. Effects of aging on the microstructure and phase transformation behavior of effects of aging on the microstructure and phase transformation behavior of Cu-Al-Mn shape memory alloy. 2021, https://doi.org/10.4028/www.scientific.net/KEM.882.21.

52. Yildiz, K., Balci, E., Akpinar, S. Quenching media effects on martensitic transformation, thermodynamic and structural properties of Cu–Al–Fe–Ti high- temperature shape memory alloy. *J. Therm. Anal. Calorim*. 2017, https://doi.org/10.1007/s10973-017-6219-2.
53. Liu, M., Zhu, J., Popovich, V.A., Borisov, E., Mol, J.M.C. Passive film formation and corrosion resistance of laser-powder bed fusion fabricated NiTi shape memory alloys. *J. Mater. Res. Technol.*, **2023**, *23*, 2991–3006, https://doi.org/10.1016/j.jmrt.2023.01.204.
54. Chu, C.L., Chung, C.Y., Chu, P.K. Surface oxidation of NiTi shape memory alloy in a boiling aqueous solution containing hydrogen peroxide. *Mater. Sci. Eng. A*, **2006**, *417*, 104–109, https://doi.org/10.1016/j.msea.2005.11.010.
55. Zhou, P., Liu, Y., Chen, Q., Li, H., Bian, R., Xu, W., Yang, Q., Liu, D. Femtosecond laser-induced hydrophobic surface of NiTi shape memory alloy and its blood compatibility. *Phys. Status Solidi.*, **2023**, *220*, 2200747, https://doi.org/https://doi.org/10.1002/pssa.202200747.
56. Wang, G., Xia, H., Huang, W., Yang, J., Liu, B., Yuan, L. Influence of milling—electrochemical polishing on corrosion resistance of niti shape memory alloy. Micromachines (Basel), **2022**, 13(12), 2204.
57. Firstov, G.S., Vitchev, R.G., Kumar, H., Blanpain, B., Van Humbeeck, J. Surface oxidation of NiTi shape memory alloy. *Biomaterials*. **2002**, *23*, 4863–4871.
58. Woodside, C.R., King, P.E., Nordlund, C. Arc distribution during the vacuum arc remelting of Ti-6Al-4V. *Metall. Mater. Trans. B* **2013**, *44*, 154–165, https://doi.org/10.1007/s11663-012-9760-1.
59. Frenzel, J., Zhang, Z., Neuking, K., Eggeler, G. High quality vacuum induction melting of small quantities of NiTi shape memory alloys in graphite crucibles. *J. Alloys Compound.*, **2004**, *385*, 214–223, https://doi.org/10.1016/j.jallcom.2004.05.002.
60. Karimi-Sibaki, E., Kharicha, A., Vakhrushev, A., Abdi, M., Wu, M., Ludwig, A., Bohacek, J., Preiss, B. Numerical modeling and experimental validation of the effect of arc distribution on the as-solidified Ti64 ingot in vacuum arc remelting (VAR) process. *J. Mater. Res. Technol.*, **2022**, *19*, 183–193, https://doi.org/https://doi.org/10.1016/j.jmrt.2022.05.036.
61. Mohd, J., Leary, M., Subic, A., Gibson, M.A. A review of shape memory alloy research, applications and opportunities. *Mater. Des.*, **2014**, *56*, 1078–1113, https://doi.org/10.1016/j.matdes.2013.11.084.
62. Santoro, M., Nicolay, O.F., Cangialosi, T.J. Pseudoelasticity and thermoelasticity of nickel-titanium alloys: a clinically oriented review. Part I: temperature transitional ranges. *Am. J. Orthod. Dentofac. Orthop.*, **2001**, *119*, 587–593, https://doi.org/10.1067/mod.2001.112446.
63. Santoro, M., Nicolay, O.F., Cangialosi, T.J. Pseudoelasticity and thermoelasticity of nickel-titanium alloys: a clinically oriented review. Part II: deactivation forces. *Am. J. Orthod. Dentofac. Orthop.*, **2001**, *119*, 594–603, https://doi.org/10.1067/mod.2001.112447.
64. Sherif, M., Ozbulut, O., La, A., Hamilton, R.F. Self-post-tensioning for concrete beams using shape memory alloys. In *ASME 2014 Conference on Smart Materials, Adaptive Structures and Intelligent Systems, SMASIS 2014*, 2014, p. 2, https://doi.org/10.1115/SMASIS20147564.
65. Restasari, A., Budi, R.S., Hartaya, K. Pseudoplasticity of propellant slurry with varied aluminium content for castability development. *J. Phys. Conf. Ser.*, **2018**, *1005*, https://doi.org/10.1088/1742-6596/1005/1/012034.

66. Ravi, V., Jog, M.A., Manglik, R.M. Effects of pseudoplasticity on spread and recoil dynamics of aqueous polymeric solution droplets on solid surfaces. *Interfacial Phenom. Heat Transf.*, **2013**, *1*, 273–287, https://doi.org/10.1615/interfacphenomheattransfer.2013010246.
67. Pogrebnjak, A., Bratushka, S., Levintant-Zayonts, N. High dose ion implantation into NiTi for improvement of pseudoplasticity and shape memory effect. *J. Nano- Electron. Phys.*, **2013**, *5*, 1–8.
68. Balestrieri, D., Philipponneau, Y., Decroix, G.M., Jorand, Y., Fantozzi, G. Pseudoplasticity of monoclinic Gd2O3. *J. Eur. Ceram. Soc.*, **1998**, *18*, 1073–1077, https://doi.org/10.1016/S0955-2219(97)00190-8.
69. Pan, Q., Cho, C. The investigation of a shape memory alloy micro-damper for MEMS applications. *Sensors*. **2007**, *7*, 1887–1900.
70. Van Humbeeck, J., Kustov, S. Active and passive damping of noise and vibrations through shape memory alloys. **2005**, *171*, https://doi.org/10.1088/0964-1726/14/5/001.
71. Akhavan, B., Mohammad, R., Kheirikhah, M. Static analysis of sandwich plates embedded with shape memory alloy wires using active strain energy tuning method. *J. Brazilian Soc. Mech. Sci. Eng.*, **2019**, *41*, 1–17, https://doi.org/10.1007/s40430-019-1666-2.
72. Menzel, A.M. Tuned, driven, and active soft matter. *Phys. Reports,* **2015**, *554*, 1–84, https://doi.org/10.1016/j.physrep.2014.10.001.
73. Liang, C., Rogers, C.A. One-dimensional thermomechanical constitutive relations for shape memory materials. *J. Intell. Mater. Syst. Struct.*, **1990**, *1* (2), 207–234, https://doi.org/10.1177/1045389X9000100205.
74. B. Reviews, Physical properties of crystals—their representation by tensors and matrices. *Phys. Bull.* **1985**, *36*, 506.
75. W.H. K.L. WolframWersing, Piezoelectricity Evolution, 2008. http://scholar.google.com/scholar?hl=en&btnG=Search&q=intitle:No+Title#0
76. Anton, S.R., Sodano, H.A. Topical review a review of power harvesting using piezoelectric materials (2003–2006). **2007**, *16*, 1–21, https://doi.org/10.1088/0964-1726/16/3/R01.
77. Katsouras, B.I., Asadi, K., Li, M., Van Driel, T.B. The negative piezoelectric effect of the ferroelectric polymer poly(vinylidene-fluoride). *Nat. Mater*. **15**, 78–84
78. Arnau, A., D. Soares, Fundamentals of piezoelectricity, In Vives, A.A. (Ed.), *Piezoelectric transducers and applications*, 2008, p. 532. https://doi.org/10.1007/978-3-540-77508-9
79. Starr, M.B., Wang, X. Coupling of piezoelectric effect with electrochemical processes. *Nano. Energy*, **2015**, *14*, 296–311, https://doi.org/10.1016/j.nanoen.2015.01.035.
80. Coutte, J. Design, production and testing of PMN–PT electrostrictive transducers. Ultrasonics, **2002**, *40*, 883–888.
81. Yang, J. *An introduction to the theory of piezoelectricity*, Springer, **2004**, 300.
82. Davoudi, S. Effect of temperature and thermal cycles on PZT ceramic performance in fuel injector applications, Master's thesis, **2012**.
83. Jaffe, B., Cook Jr, W.R., Jafee, H. Interpretation of some experimental results. In *Piezoelectric Ceramics*, **1971**, pp. 237–251. https://doi.org/10.1016/B978-0-12-379550-2.50014-4.
84. Newnham, R.E., Sundar, V., Yimnirun, R., Su, J., Zhang, Q.M., Park, U.V., Pennsyl, V., May, R.V. Electrostriction : nonlinear electromechanical coupling in solid dielectrics. *J. Phys. Chem. B*, **1997**, *5647*, 10141–10150.
85. Safari, A., Jadidian, B., Akdogan, E.K. Piezoelectric composites for transducer applications. *Compr. Compos. Mater.*, **2000**, 533–561, https://doi.org/10.1016/b0-08-042993-9/00095-4.
86. Dao, D.V., Nakamura, K., Bui, T.T., Sugiyama, S. Micro/nano-mechanical sensors and actuators based on SOI-MEMS technology. *Adv. Nat. Sci. Nanosci. Nanotechnol.*, **2010**, *1*, https://doi.org/10.1088/2043-6254/1/1/013001.

87. Almeida, H., Amaral, M.H., Lobão, P. Temperature and pH stimuli-responsive polymers and their applications in controlled and selfregulated drug delivery. *J. Appl. Pharm. Sci.*, **2012**, *2*, 01–10, https://doi.org/10.7324/JAPS.2012.2609.
88. Kocak, G., Tuncer, C., Bütün, V. PH-responsive polymers. *Polym. Chem.*, **2017**, *8*, 144–176, https://doi.org/10.1039/c6py01872f.
89. Chaturvedi, K., Ganguly, K., Nadagouda, M.N., Aminabhavi, T.M. Polymeric hydrogels for oral insulin delivery. *J. Control. Release.*, **2013**, *165*, 129–138, https://doi.org/10.1016/j.jconrel.2012.11.005.
90. Arbabi, N., Baghani, M., Abdolahi, J., Mazaheri, H., Mosavi-Mashhadi, M. Study on pH-sensitive hydrogel micro-valves: a fluid–structure interaction approach. *J. Intell. Mater. Syst. Struct.*, **2017**, *28*, 1589–1602, https://doi.org/10.1177/1045389X16679020.
91. Van Der Schueren, L., de Clerck, K. The use of pH-indicator dyes for pH-sensitive textile materials. *Text. Res. J.*, **2010**, *80*, 590–603, https://doi.org/10.1177/0040517509346443.
92. Ferrara, M., Bengisu, M. Materials that change color: smart materials, intelligent design (Springer Briefs in applied sciences and technology). 2013. http://www.amazon.com/exec/obidos/redirect?tag=citeulike07-20&path=ASIN/3319002899.
93. Halsey, T.C. Electrorheological fluids, *Science*, **1992**, *258*(5083), 761–766
94. Wen, W., Huang, X., Sheng, P. Electrorheological fluids: structures and mechanisms, *Soft Matter.*, **2008**, *4*, 200, https://doi.org/10.1039/b710948m.
95. Ashour, O., Rogers, C.A., Kordonsky, W. Ashour1996.Pdf. *J. Intell. Mater. Syst. Struct.*, **1996**, *7*, 123–130.
96. Tao, R. Super-strong magnetorheological fluids. *J. Phys. Condens. Matter.*, **2001**, *13*, https://doi.org/10.1088/0953-8984/13/50/202.
97. De Vicente, J., Klingenberg, D.J., Hidalgo-Alvarez, R. Magnetorheological fluids: a review. *Soft Matter.*, **2011**, *7*, 3701–3710, https://doi.org/10.1039/c0sm01221a.
98. Genc, S. Synthesis and properties of magnetorheological (MR) fluids, 2003. http://d-scholarship.pitt.edu/8924/1/genc12-20.pdf.
99. Taylor, P., Udd, E. Fiber and integrated optics. *Opt. Fib. Sensors*. **2006**, 37–41, https://doi.org/10.1080/01468039208204198
100. Udd, E. An overview of fiberoptic sensors, *Rev. Sci. Instrum.* **1997**, *4015*, https://doi.org/10.1063/1.1145411
101. Butter, C.D., Hocker, G.B. Fiber optics strain gauge, *Appl. Opt.*, **1978**, *17*, 2867–2869.
102. Culshaw, B., Kersey, A. Fiber-optic sensing: a historical perspective. *J. Lightwave Technol.* **2008**, *26*, 1064–1078.
103. Chtcherbakov, A.A., Swart, P.L., Spammer, S.J., Mach–Zehnder and modified Sagnac-distributed fiber-optic impact sensor. *Appl. Opt.* **1998**,*37*, 3432–3437, https://doi.org/10.1364/AO.37.003432.
104. Chen, W.C. Some experimental investigations in the drilling of carbon fiber-reinforced plastic (CFRP) composite laminates. *Int. J. Mach. Tools Manuf.*, **1997**, *37*, 1097–1108, https://doi.org/10.1016/S0890-6955(96)00095-8.
105. Ning, F., Cong, W., Hu, Y., Wang, H. Additive manufacturing of carbon fiber-reinforced plastic composites using fused deposition modeling: effects of process parameters on tensile properties. *J. Compos. Mater.*, **2017**, *51*, 451–462, https://doi.org/ 10.1177/0021998316646169.
106. Corres, J.M., Arregui, F.J., Matias, I.R. Design of humidity sensors based on tapered optical fibers. *J. Light. Technol.*, **2006**, *24*, 4329–4336, https://doi.org/10.1109/JLT.2006.883668.

107. Wang, Q., Zhao, W.M. A comprehensive review of lossy mode resonance-based fiber optic sensors. *Opt. Lasers Eng.*, **2018**, *100*, 47–60, https://doi.org/10.1016/j.optlaseng.2017.07.009.
108. Zamarreño, C.R., Hernáez, M., Del Villar, I., Matías, I.R., Arregui, F.J., Optical fiber pH sensor based on lossy-mode resonances by means of thin polymeric coatings. *Sensor. Actuat. B Chem.*, **2011**, *155*, 290–297, https://doi.org/10.1016/j.snb.2010.12.037.
109. Wang, H., Jiang, L., Xiang, P. Improving the durability of the optical fiber sensor based on strain transfer analysis. *Opt. Fiber Technol.*, **2018**, *42*, 97–104, https://doi.org/10.1016/j.yofte.2018.02.004.
110. Wang, C., Hu, Y., Liu, Y., Shan, Y., Qu, X., Xue, J., He, T., Cheng, S., Zhou, H., Liu, W., Guo, Z.H., Hua, W., Liu, Z., Li, Z., Lee, C. Tissue-adhesive piezoelectric soft sensor for in vivo blood pressure monitoring during surgical operation. *Adv. Funct. Mater.*, **2023**, *2303696*, 1–10, https://doi.org/10.1002/adfm.202303696.
111. Mokhtari, F., Cheng, Z., Wang, C.H., Foroughi, J. Advances in wearable piezoelectric sensors for hazardous workplace environments. *Glob. Chall.*, **2023**, *7*, 2300019, https://doi.org/10.1002/gch2.202300019.
112. Duan, S., Wu, J., Xia, J., Lei, W. Innovation strategy selection facilitates high-performance flexible piezoelectric sensors. *Sensors (Switzerland).*, **2020**, *20*, https://doi.org/10.3390/s20102820.
113. Du, Y., Wang, R., Zeng, M., Xu, S., Saeidi-Javash, M., Wu, W., Zhang, Y. Hybrid printing of wearable piezoelectric sensors. *Nano Energy*. **2021**, *90*(Part A), 106522, https://www.sciencedirect.com/science/article/pii/S2211285521007758
114. Zhang, S., Yu, F. Piezoelectric materials for high temperature sensors, *J. Am. Ceram. Soc.*, **2011**, *94*, 3153–3170, https://doi.org/10.1111/j.1551-2916.2011.04792.x.
115. Ju, M., Dou, Z., Li, J.W., Qiu, X., Shen, B., Zhang, D., Yao, F.Z., Gong, W., Wang, K. Piezoelectric materials and sensors for structural health monitoring: fundamental aspects, current status, and future perspectives. *Sensors*, **2023**, *23*,543. https://doi.org/ 10.3390/s23010543.

CHAPTER 3

EXPLORING THE POTENTIAL OF SMART MATERIALS: AN OVERVIEW OF PROPERTIES AND APPLICATIONS

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ABSTRACT

A material that instantly responds to the environment on its own is referred to as smart materials (SMs). These materials reactions result in some changes in volume, color, viscosity, and odor. The change in stress, temperature, electric current, pH value, or magnetic field may cause this kind of reaction. The ability of the behavior of SMs to return to the initial state after the stimulus has been impassive is a key characteristic of their behavior. Since its beginnings, material science has undergone substantial development. From the use of inert structural materials to materials designed with a particular function, active or adaptive materials, and ultimately SMs with more sophisticated recognition, discrimination, and response capabilities. To encompass this final transformation, new SMs and alloy materials must

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satisfy a number of basic fundamentally important requirements. When it interacts with stimuli under controlled circumstances and performs its functions in recent years. In order to use SMs effectively in common and in mechatronic applications, they must have certain properties. SMs have developed a wide variety of applications as a result of their distinctive properties based on the properties.

3.1 INTRODUCTION

Diverse materials were used by humans in the past, and as a result, their standard of living improved. These were divided even after civilizations based on the discovery of materials such as Stone Age (first age). Due to the durability and hardness of bronze, the Bronze Age (also known as the Second Age) was the most revolutionary period. Science and technology have advanced significantly in the last two decades in terms of analyzing novel materials. They are divided mainly into four categories which are

1. Ceramic materials
2. Polymer materials
3. Metals
4. Smart materials (SMs)

Among them, SMs are becoming more popular because of their various applications compared to other standard materials [1].

SMs have been defined as substances that can replace their behavior in a consistent way in response to particular stimuli that are changed. These are more popular as compared to other standard materials due to their wide range of applications. These materials can alter their shape when they are kept near a magnet just by append some external heat or can commute their phase suddenly. SMs have properties that may be changed by stimuli such as temperature, pressure, humidity, pH, electric/magnetic fields, etc.

Intelligent practises include the ability to revert to the original state once the stimulus has been detached. There are numerous groups of SMs, each displaying distinct abilities that can be used in a variety of high-tech and everyday applications. These contain pH-sensitive materials, shape memory alloys (SMAs), piezoelectric materials, magneto-rheological and electrostrictive materials, electrorheological materials, magnetostrictive materials, and chromic materials (such as photochromic, thermochromic, electrochromic, and magnetochromics), which translate their color interaction to various stimuli. Existing SMs include piezoelectric materials that generate a voltage when stressed or the opposite when relaxed. Due to amazing and superintended structural changes, thermo-responsive materials like SMAs or shape memory polymers can accommodate a variety of shapes at incompatible temperatures. Materials called pH intuitive polymers break down when the pH of the surrounding media changes. Gels made of polymer have a lot of potential for intelligent behavior [2]. The SMs listed above are important because some of them are attracting more attention from researchers as a result of their potential use in delicate industries like medicine, automobile engines, robots, and extremely compressed devices [3, 4].

A smart nanomaterial (SNMs) has been emerged as one of the extraordinary materials to the contemporary world due to their irregular thermal, electronic, optical, and mechanical properties. It has unique properties to make them striking candidates for pharmaceutical analysis, which basically determines the quality of drug products via analytical chemistry [5]. Distinguishing smart and nanomaterials, the SMs perform both sensing and actuating operations, whereas many nanomaterials are capable of self-assembly [6].

SMs offer noticeable and substantial reactions to interchange their backgrounds or to exterior their stimuli nature. Such SMs are also exclaimed *intelligent or responsive* due to their distinctive self-adaptability, sensing, or memory capabilities. Due to these remarkable properties, SMs are gaining considerable importance in many industries and can have a profound impact on the environment [7, 8].

To achieve a specific objective for a particular function, materials have to satisfy some technical properties such as thermal processing, welding abilities, mechanical and behavioral characteristics, technological properties encompassing manufacturing, forming, welding abilities, waste level, workability, automation and repair capacities, economic criteria, related to raw material and production costs, supply expenses and availability; environmental characteristics, including features such as toxicity and pollution; and sustainable development criteria, implying reuse and recycling capacities [9].

Surveillance at the most elementary stage in materials includes three functions: (1) sensor function, (2) effector or actuator function, and (3) processor function. These three functions have been supported by even more primitive functions such as the energy conversion and supply function, the systematic information transfer function, and functions and structures at the most fundamental levels in physics and chemistry [10].

3.2 NEW MATERIAL REQUIREMENTS

There are varieties of nanomaterials have been developed over the past years which could be used as SMs that showed intellectual performance during changes produced in the environment such as metallic nanomaterials, graphene, carbon nanomaterials (CNM), and electrospun nanofibers [11].

The SNMs have been categorized based on their interconnection to the environment; (1) environment-notified nanoparticles and (2) environment-perceptive nanoparticles. The high-quality primed nanoparticles recognize and react to their environment. Any pathological condition shows a transpose in biochemical possessions such as pH, redox potential, enzymatic activity, and homeostatic pathways. These resources have been utilized to immobilize nanoparticles which are superintended to the preceding pathological circumstances. The second class of responsive nanoparticles manipulates the host environment by the administration of radiations (X-rays, infrared, and heat), drugs, and interactions between nanoparticles & nanoparticle and nanoparticles to enable host-nanoparticle [5]. A contemporary favorable field of this research is the conspiring of SNMs whose chemical structure or possessions are receptive to the bio-catalytic gesture of enzyme. Enzymes have played a vital role in all biological and metabolic processes and their dysregulation is a characteristic of many ailments. Thus, the SNMs can sense these enzymes in the host environment and act as a promising tool for diagnostic and therapeutic applications [12].

There are several categories of SMs available, each material exhibiting particular properties (Figure 3.1), which have been harnessed by a variety of high tech and everyday applications. Recent examples of SMs include self-healing polymers that release healing agents upon structural damage, an electronic paper display, whose ink appears or disappears depending on electrical charge, and meta-materials that serve as an *invisibility cloak* to make objects invisible at a particular wavelength [13].

3.2.1 NEEDS OF SMART MATERIALS

SMs have adaptable potential to environmental cues. High-speed SMs have been used throughout the entire structure as building media. Compared to other conventional materials, these materials promise easier, cheaper, and more durable construction. These SMs offer a significant chance for the design of new structures as well as the restoration of old, damaged structures. The nature of SMs has reorganized their use in a variety of infrastructure systems, and they are also expanding extraordinarily quickly. The most significant developments are anticipated in new composite materials, particularly in applications related to electronics, optics, and biomedicine [14].

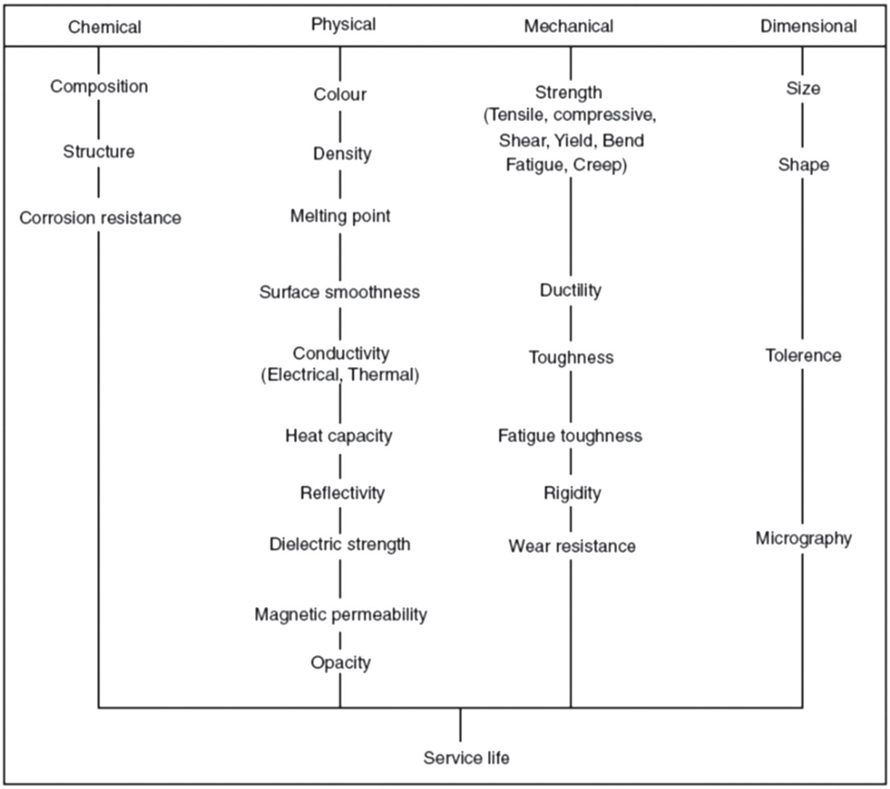
Chemical
Physical
Mechanical
Dimensional
Composition
Structure
Corrosion resistance
Colour
Density
Melting point
Surface smoothness
Conductivity (Electrical, Thermal)
Heat capacity
Reflectivity
Dielectric strength
Magnetic permeability
Opacity
Strength (Tensile, compressive, Shear, Yield, Bend Fatigue, Creep)
Ductility
Toughness
Fatigue toughness
Rigidity
Wear resistance
Size
Shape
Tolerence
Micrography
Service life

FIGURE 3.1 Required properties of materials. ⏎

1. Technical properties: These comprise mechanical characteristics like plastic flow, fatigue, and yield strength, as well as behavioral characteristics like damage tolerance and electrical, heat, and fire resistance.
2. The technical attributes encompass the following: waste management, workability, automation, welding, forming, manufacturing, thermal processing, and repair capabilities.

3. The economic criteria comprised costs related to raw materials and production, availability, and supply.
4. Environmental features: These comprise things like toxicity and pollution.
5. Reusing and recycling materials is a prerequisite for sustainable development. If the novel material's sensing and actuation capabilities are added to the list, it is considered an SM.

3.3 THE NATURE OF SMART MATERIALS

The common structural and efficient materials are carried by SMs, which are new prompting materials. SMs are materials with comprehensive capabilities to external stimuli, like loads or environment, and the capacity to change their physical properties in a specific way in response to those inputs.

The stimuli may include chemicals, hydrostatic pressure, electric and magnetic fields, moisture, stress, pressure, temperature, pH, and nuclear radiation.

These are classified into active and passive based on the account of their characteristics (Figure 3.2). It has been noted by Scientist Fairweather (1998) that active smart materials (ASMs) can alter their geometric or material properties when subjected to electric, thermal, or magnetic fields. AS materials include piezoelectric materials, SMAs, ER fluids, and magnetostrictive materials. Passive smart materials (PSMs) are defined as materials which lack the potential capacity to convert energy. Acquiescent SM is a good example for fiber optic material. Such materials can behave as sensors but not as actuators or transducers [15].

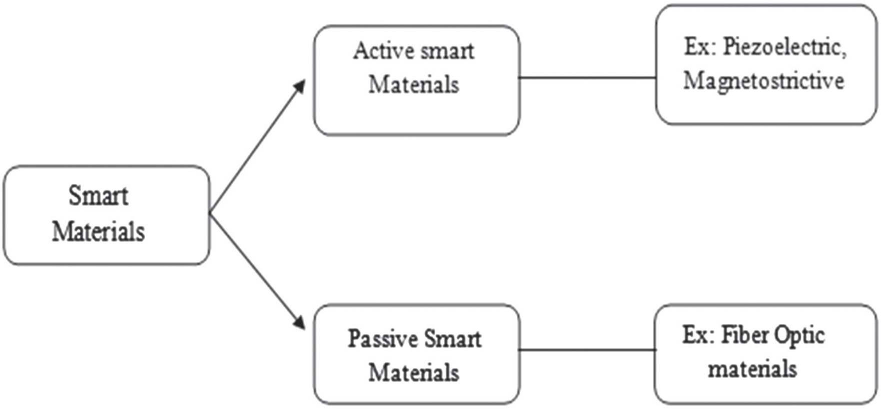
Smart Materials
Active smart Materials
Ex: Piezoelectric, Magnetostrictive
Passive Smart Materials
Ex: Fiber Optic materials

FIGURE 3.2 Types of smart materials. ⏎

These SMs possess environmental stimuli with particular alterations in specific variables. For that reason, they are actually referred as approachable materials. On account of the variation in some extrinsic conditions, SMs can alter their characteristics (mechanical, electrical, and appearance), structure, composition, or functions. Most of the SMs are implanted in systems whose potential effects can be drastically altered to meet performance needs.

3.4 PROPERTIES OF SMART MATERIAL

Self-healing and self-adaptability by changing its chances more than composites and ceramics are two characteristics of SMs. The smart structure shown in Table 3.1, which is composed of one or more SMs, actuators, and sensors, has sparked a lot of interest in this area. The current generation of SMs and their structures share a number of traits, including:

1. Sensors that are reinforced inside a structural material or that are bonded to its surface.

TABLE 3.1 Material Classes of Sensor and Actuator ⏎

Variables	Material Class	Stimulus	Response
Sensors	Pyroelectrics	Temperature change	Electric polarization
	Piezoelectrics	Mechanical strain	Electric polarization
	Electrostrictors	Mechanical strain	Electric polarization
	Magnetostrictors	Mechanical strain	Change in magnetic field
	Electroactive polymers	Mechanical strain	Electric polarization
	Electroluminescent	Electric field	Light emission
	Photoluminescent	Incident light	Light emission
	Electrochromic	Electric field	Color change
Actuators	Piezoelectrics	Electric current	Mechanical strain
	Electrostrictors	Electric current	Mechanical strain
	Magnetostrictors	Electric field	Mechanical strain
	Shape memory alloys	Temperature change	Mechanical strain
	Electroactive polymers	Electric field	Mechanical strain
	Electrorheological fluids	Electric field	Viscosity change
	Magnetorheological fluids	Magnetic field	Viscosity change

2. Actuators are reinforced by the structural material or attached to the material's surface layer. When exposed to an external stimulus, such

as an electric current, these actuators automatically jump, altering their geometric configuration, hardness, and energy-dissipation characteristics (Figure 3.3).

3. Control capabilities permit the behavior of the material to respond to an external stimulus according to a prescribed functional relationship or control algorithm [16].

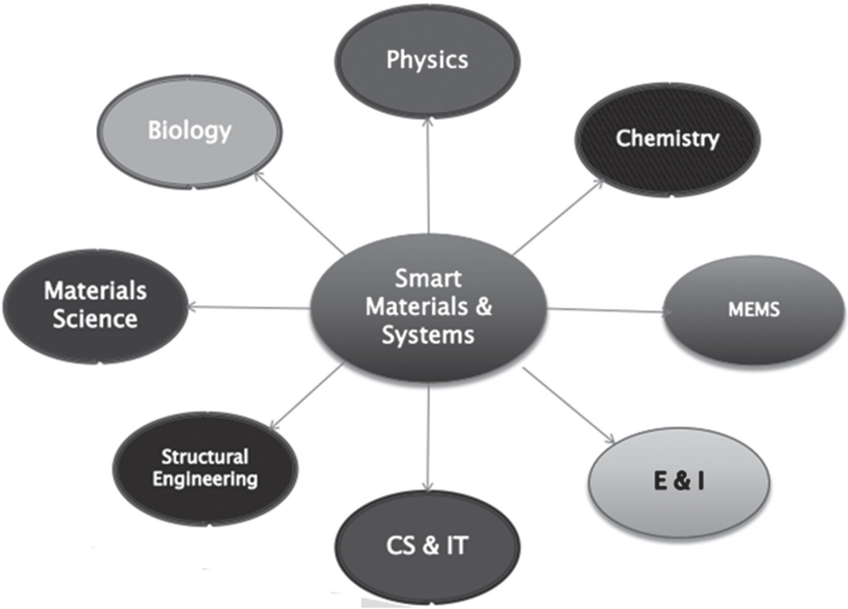

FIGURE 3.3 Interdisciplinary natures of SMs. ⏎

These SMs can perceive a wide range of applications, such as those in civil engineering, aerospace, electronics, and mechatronics, because of their varied responses to external stimuli. The broad range of these applications allows for the infeasible efficient resolution of engineering issues as well as the potential for the development of novel, profit-generating products. The ability of SMs structures to function in every area of science, engineering, and technology is their most outstanding quality. Legislation, efforts to reduce waste, and the desire for a better quality of life are some of the factors driving investment in research and development [17].

These SMs must now be used in multidisciplinary constructions because they are susceptible to changes in their characteristics when exposed to extrinsic stimuli. Their reversibility, demonstrated by their capacity to sense, heal, and adjust to shifting environmental conditions, makes them one of the extraordinary materials. These variables include but are not limited to temperature, mechanical strain, hydrostatic pressure, magnetic field, electric current, pH, and chemical reaction. These properties can lead to change in humidity, size, scent, color, and flow of viscosity [18]. SMs have a wide range of applications in alloys, composites, gels, and polymers and have been identified for enormous applications from aerospace industry to pharmaceutical technologies. These SMs can be designed with various responses and actuation mechanism based on the requirements of applications [19].

3.5 TYPES OF SMART MATERIAL

External stimuli such as pH, temperature, moisture, electric field, and magnetic field can significantly and controllably alter the properties of SMs. Material intelligence has been defined by its self-adaptability, sensing, and repairing capabilities. There are numerous uses for these SMs in all fields of science and engineering.

The distribution of these materials will likely be influenced by the common denominator of the mechanical or structural system's operating environment, despite the differences in the electrical and electronic applications for these new generations of SMs. Based on different types of SMs different properties are available and some of them are mentioned below (Figure 3.4).

i. *Piezoelectric:* The terms piezo and electric are first divided to create these. The Greek word *piexein*, which means to press down *tightly or squeeze*, is where the word *piezo* originates. The meaning of *squeeze electricity* is created by arranging *piexein* with electric. The Curie brothers conducted the first studies on this intriguing phenomenon, known as piezoelectricity, between 1880 and 1881. It applies mechanical stress to the materials, which results in the generation of an electric current. Piezoelectric microphones convert sound waves' pressure into an electrical signal.

   The piezoelectric effect exists in a number of naturally occurring crystals such as quarts, tourmaline, and sodium potassium tartrate [20, 21]. The piezoelectric materials have the potentiality to create voltage when pressure is solicited and indistinguishable process can take place in a regenerable manner. This material can be used to create structures that can flex, expand, and contract (Figure 3.5).

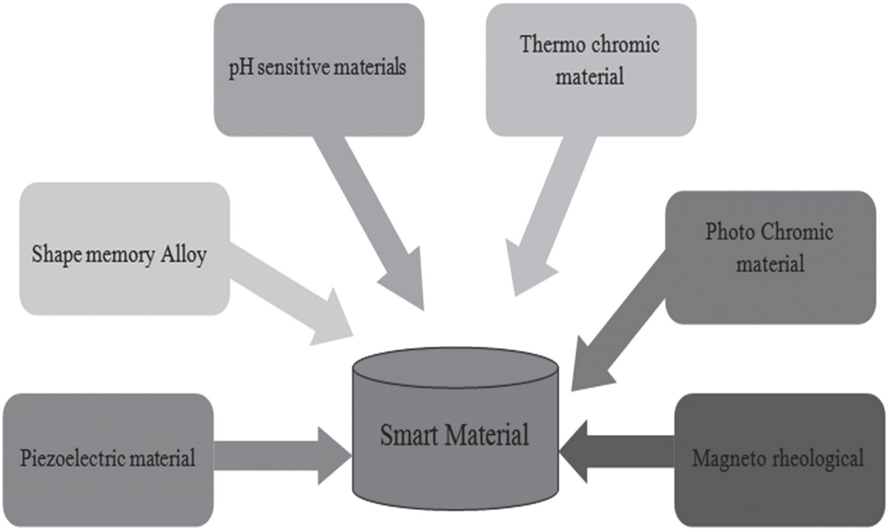
pH sensitive materials
Thermo chromic material
Shape memory Alloy
Photo Chromic material
Smart Material
Piezoelectric material
Magneto rheological

FIGURE 3.4 Classification of smart materials. ⏎

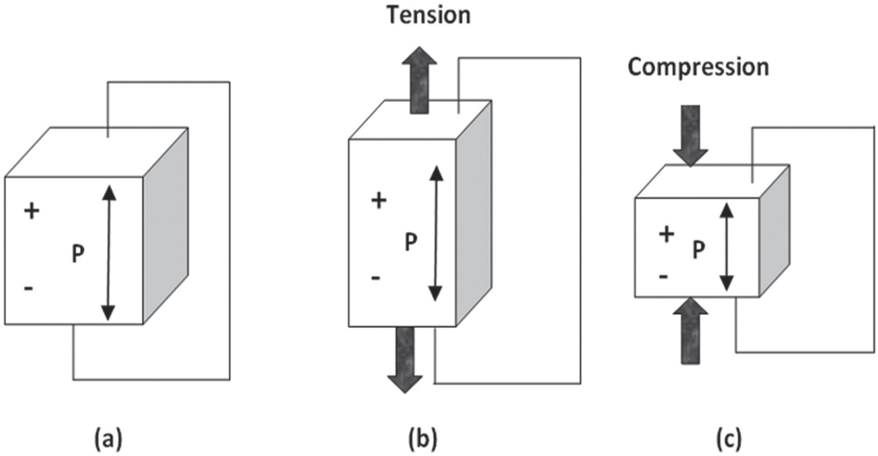
Tension
Compression
+
P
-
+
P
-
+
P
-
(a)
(b)
(c)

FIGURE 3.5 Schematic representations of piezoelectric materials. ⏎

Example: Quartz, $BaTiO_3$, $GaPO_4$

Applications of the piezoelectric materials:

- Used in ink jet printers
- Used in sonar
- Used in medical diagnostics

- Used in high-frequency stereo speakers
- Used in computer keyboards
- used in microphone and
- Used in airbag sensors

ii. *Shape memory alloy (SMA):* After deformation when heated these particulars, they look back on their authentic shape and came back to their genuine shape. These SMA details have a minimum of two basic, incompatible stages that can be switched between by varying temperature or stress. These shape changes occur between the two phases of austenite and martensite. The austenite phase is stable at higher temperatures, while the martensite phase is stable at lower temperatures. These materials essentially exist between two phases. This process, known as shape memory modification, caused changes to the solid's atomic structure and microstructure (Figure 3.6).

iii. Some uses make use of shape memory stents, which are tubes that are inserted into arteries and expand to enhance blood flow when heated to body temperature.

Examples of SMA: NiTiNOL (thermal), NiMnGa, FePd, Terfenol-D (Magnetic) CuZnSi, CuZnAl, CuZnGa, and CuZnSn (actuator)

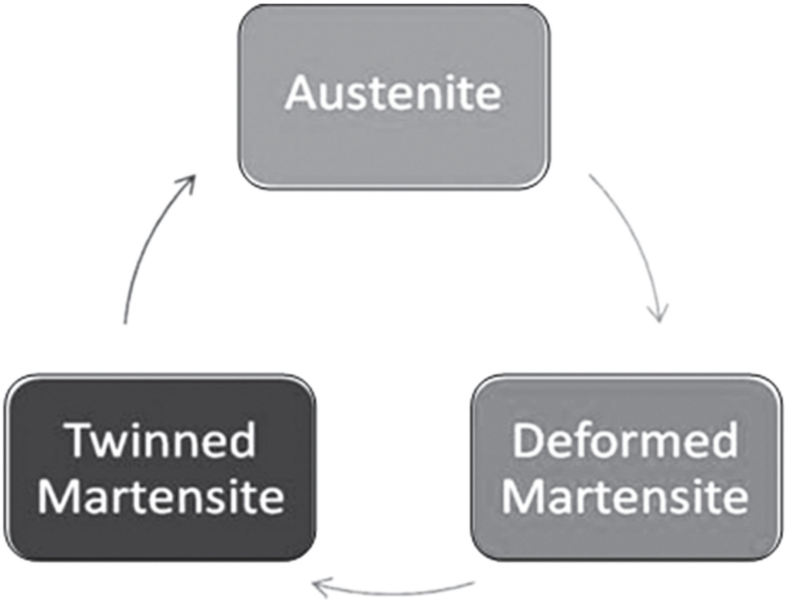

FIGURE 3.6 Forms of shape memory alloy (SMA). ⏎

In many fields, nickel–titanium alloys are regarded as potential shape memory materials. Following its first detection during its laboratory synthesis (Nickel Titanium Naval Ordinance Laboratory), this group of family of nickel–titanium alloys is known as Nitinol. Nitinol has been applicable in military, medical, safety, and robotics applications [22].

Applications of the SMA:

- Aeronautical applications
- Surgical tools
- Muscle wires and
- Thermostats

iv. *Thermo chromic:* It indicates that they alter their color in response to temperature changes. When used with bath plugs, which when heated to a high temperature change the color of the water. By raising the temperature to a certain range, thermochromic details colors have been changed. It can be produced using certain semiconductor, metal, and liquid crystal compounds. Without changing the chemical compound, this temperature can change the crystal structure, the stereoscopic position of atoms, or the arrangement of atoms in molecules. These materials' various applications in incompatible fields are also numerous. Thermo strips can be used as temperature gauges, particularly for detecting fever.

New layout possibilities for instrumentation, low-level lighting systems, etc. have been created by an advanced type of phosphorescent pigment that can emit light for up to ten hours.

v. *Photochromic:* The colors of these materials vary depending on the lighting. These chromic materials can emit specific colors based on the intensity of a given light range, and they are usually very sensitive to visible and ultraviolet light. Both organic and inorganic materials can exhibit photochromic properties. When photochromic eyewear comes into contact with solar radiation, their transparency can be reduced. Additionally, some textile fabrications and protective clothing for the military use photochromic materials. One application is for security ink sand dolls that "tan" in the sun.

When the photochromic lenses are in contact to UV radiation they become dark. They can return back their original state after releasing the contact of UV radiation. It has been made of either glass or plastic. Spiro pyranes, naphtha pyranes, spiro oxazines, chromenes, spiro dihydro indolizines, fulgides, diaryl ethenes, bacteriorhodopsin and azo compounds are the most significant photochromic materials [23].

Applications of photochromic:

- Used in sun glasses
- Used in supramolecular chemistry
- Used in data storage and also
- In novelty items

vi. pH-sensitive materials

These materials are SMs having the characteristics to color change during the change of the acidity of liquids. When these materials are mixed with paint they can indicate the corrosion tendency [24].

The pH of the surrounding medium can change and cause polymers that are sensitive to it to enlarge. Color changes in other substances can occur due to variations in pH, light, or applied voltage. Among the most well-known examples of this type of sunglasses are those that darken in direct sunlight. There are two different types of pH-sensitive materials: those that have basic groups (–NH_2) and swell in acidic pH and those that have acidic groups (–COOH, SO_3H) [2].

Applications of pH sensitive materials:

- Used in controlled drug delivery systems
- Used in bio-mimetic responsive plasmonics

vii. Magnetorheological: It is a substance that resembles fluid and solidifies in the presence of a magnetic field. It can be utilized to create dampers that reduce vibration. To lessen the negative effects, these materials have been used in the construction of buildings and bridges. High winds or earthquakes are two examples of magnetorheological materials. An easy magnetorheological fluid (MRF) is made up of motor oil and iron powder. An interesting modification of magnetorestrictive fluids is a family of elastomeric matrix composites reinforced with iron particles. Thermal curing of the elastomers is achieved by aligning the iron particles into chains using a strong magnetic field. These chains of iron particles were locked into place within the composite through the cross-linked network of the cured elastomer [25].

Applications of magnetorheological material:

- Used in high-power sonar transducers

- Motors (e.g., car shocks, hydraulic actuators, engine mounts made to reduce noise, washing machine vibration damping, and surface polishing of machine parts)
- Prosthetic limbs, exercise equipment

3.6 APPLICATIONS OF SMART MATERIALS

Because of how differently they react to changes in the environment, SMs are used in a variety of settings, including light, temperature, electricity, and pressure. The key focus of SM's work is to solve engineering problems with impractical efficiency and create opportunities for the development of new products (Figure 3.7). The different areas of application can be in our day-to-day life like aerospace, civil engineering mechatronics, and some of the applications of SMs are briefly discussed below [26].

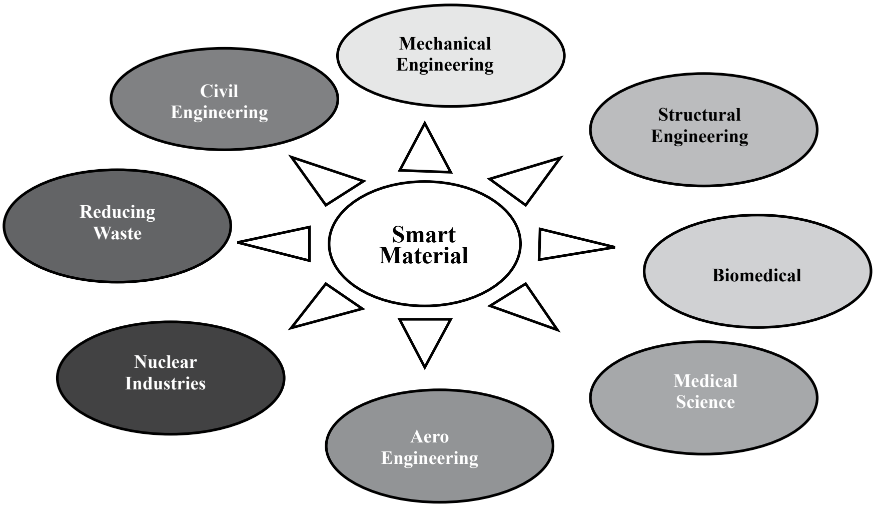
Mechanical Engineering
Civil Engineering
Structural Engineering
Reducing Waste
Smart Material
Biomedical
Nuclear Industries
Medical Science
Aero Engineering

FIGURE 3.7 Applications of various fields of smart materials. ⏎

3.6.1 CIVIL ENGINEERING

Smart bricks consist of sensors, some wireless communication devices and signal processors to measure hidden stresses, or damage after natural disaster such as earthquakes. A number of different sensors are also used to measure the force, stress and detecting the humidity, moisture, and sound. In a smart building temperature monitoring sensors are used to collect the information regarding the safety of building related to the fire [14].

3.6.2 MECHANICAL ENGINEERING

Leaf springs are made up of some composite materials of SMA. SMAs can easily regain their original property that's why it has been used in the leaf springs. SMAs have the ability to bear the high stresses and toughness so that leaf springs prevent the passengers from shock. In any critical conditions, if leaf spring deformed or broke down then it can easily regain its original properties by introducing the SMAs after heating.

3.6.3 STRUCTURAL ENGINEERING

In the discipline of structural engineering, SMs are demonstrating typical behavior. By keeping an eye on the structures created by civil engineers, the durability can be assessed. To adjust to changes in their surroundings, they can move, vibrate, and display a wide range of other reactions. Such adaptable materials can be used to control the aeroelastic shape of an aeroplane wing, lightweight structures, and satellite vibration to reduce drag and improve operational efficiency. Smart structures are also being developed to monitor the structural integrity of aircraft and spacecraft.

3.6.4 BIOMEDICAL APPLICATIONS

Research in the areas of biomedicine and medical diagnostics still needs to be done in large quantities. Certain materials, like polyelectrolyte gels, which contain a polymer matrix that has been swollen with an appropriate solvent and can expand or contract in response to an electric field or other stimulation process, are being tested for use in artificial muscle applications. Furthermore, the materials' potential for use as a drug delivery system may stem from their biodegradability.

3.6.5 MEDICAL SCIENCE

Different surgical tools made from SMA are used in keyhole surgery. Because it has special features like it can be easily bent in a particular shape for individual patient and after every individual usage it can be return to their original shape. The temperature of the mouth activates the SMA material that is used to form the teeth into the desired shape. The SMA exerts enough force as it contracts to move the teeth slowly and gradually [27–32].

3.6.6 AEROSPACE ENGINEERING

The aerospace industry is highly interested in SMs due to light weight, reduction in the complexity of product, and effective material properties. In the aircraft wings for controlling the flaps on the trailing edge the wire made of SMA is used which reduces the component size, complexity, functionality, reliability, design flexibility, and reduce weight. While on the other hand, in conventional method, it has been controlled by the hydraulic systems.

3.6.7 NUCLEAR INDUSTRIES

It offers improved performance, lowered personal exposure, new opportunities in the nuclear industrial sector, and reductions in life cycle costs for safety enhancement. However, testing of SMs faces a special challenge because of the qualification, use, and radiation environments related to nuclear operations. However, using SMs in nuclear facilities necessitates understanding how radiation-sensitive materials react to exposure and how the radiation dose affects these reactions.

3.6.8 STEALTH APPLICATION

In this stealth technology, the object is to operate without changing the indication of their presence or hide to enemy force which is achieve by make them less visible to the detection methods such as inferred, radar, and sonar. 1958 during Cold War the development of stealth technologies in the US began. The bomber B-2 and fighter jet F-117 are very good examples of this technology.

3.6.9 THERMAL MITIGATION

It is the thermal property which enables the material to make them utilizable up to ultrahigh temperature such as above 135°C by transforming their composition.

3.6.10 REDUCING WASTE

The fastest-growing component of household waste, electronic waste, now occupies the entire planet. The synthesis and disposal process itself must first remove wastes, hazardous materials, and recyclable materials. The use of SMs helps to automate the manual disassembly process, which is very time-consuming and expensive. Shape memory materials have recently been used to create fasteners that have the ability to self-release when heated. Once the fasteners have been removed, the product can be shaken to separate the parts. Products could be taken apart in a hierarchical fashion, allowing materials to be automatically sorted using temperature-sensitive fasteners.

3.7 ADVANTAGES AND DISADVANTAGES OF SMS

These resources are likely to be humanity's most innovative gateway to making a significant step toward a hopeful future. The widest variety of SMs will rule this century more than any other. The benefits of SMs are listed below.

They can adapt to their surroundings on their own, are highly sensitive to stimuli, and react quickly to various situations. When compared to other automotive systems, they are smaller and use less energy.

One of the biggest obstacles to these SMs' applications is their nonlinear nature. Some of the disadvantages of SMs are given below

- Strain outputs
- Limited blocking forces
- The costs of preparations are comparably high
- Sensitivity to harsh environmental conditions
- Dropping people out of the labor
- Nonbiodegradable material
- Environmental pollution
- Highly expensive to synthesize
- The long-term effects are unknown
- Global disaster
- They cannot operate in all temperatures
- Additionally, SMs are becoming worn out, corroded, and losing their functionality.

3.8 CONCLUSION

The SMs are used in many applications such as to generate electricity or to maintain cars and also are used in various applications. The novelty of this technology of SMs is a highly multidisciplinary field by its nature. It is used in starting from the field of entire science and engineering fields like aeronautics and mechanical engineering field. The SMs field and its structures is a thoroughly multidisciplinary field such as science, engineering & technology and also it merge the entire knowledge of science and engineering. Human ingenuity and inventiveness are used to advance human society by creating things like safer automobiles, self-repairing water pipes, more comfortable aircraft, etc. It needs to change the traditional material with the developments of these technologies that possess smartness and intelligence. There are various types of SMs are available but still lots of research work is needed on these materials to make them familiar in the entire field [33].

It is very necessary to develop the next generation SMs to obtain from natural resources so as to hold sustainability above SMs characteristics of the materials [9]. After more research and development, SMs have shown promising characteristics and will unquestionably be preferred for use in a variety of applications.

KEYWORDS

- **shape memory alloy**
- **smart materials**
- **smart behavior**
- **mechatronics**

REFERENCES

1. Bahl, S., Nagar, H., Singh, I., Sehgal, S. Smart materials types, properties and applications: a review. *Mater. Today,* **2020**, *28*, 1302–1306.
2. McCabe, J.F., Yan, Z., Al Naimi, O.T., Mahmoud, G., Rolland, S.L. Smart materials in dentistry—future prospects. *Dent. Mater. J.,* **2009**, *28*(1), 37–43.

3. Qader, I.N., Kök1, M., Dagdelen, F., Aydogdu, Y. A review of smart materials: researches and applications. *El-Cezeri J, Sci. Eng.*, **2019**, *6*(3), 755–788.
4. Shanthi, M., Soma Sekhar, E.V., Ankireddy, S. Smart materials in dentistry: think smart. *J. Pediatr. Dent.,* **2014**, *2*(1), 1–4.
5. Sharma, D., Chaudhery, M.H. Smart nanomaterials in pharmaceutical analysis. *Arab J. Chem.,* **2020**, *13*(1), 3319–3343.
6. Ghareeb, N., Farhat, M. Smart materials and structures: state of the art and applications. *Nano Res. Appl.,* **2018,** *4*(2:5), 1–5.
7. Soto, F., Karshalev, E., Zhang, F., de Avila, B.E.F., Nourhani, A., Wang, J. Smart materials for microrobots. *Chem. Rev.,* **2022**, *122*(5), 5365–5403.
8. Aizawa, S., Kakizawa, T., Higasino, M. Case studies of smart materials for civil structures. *Smart Mater. Struct.,* **1998,** *7*, 617–626.
9. Kim, H.C., Mun, S., Ko, H.-U., Zhai, L., Kafy, A., Kim, J. Renewable smart materials. *Smart Mater. Struct*., **2016**, *25*, 073001.
10. Takagi, T. A concept of intelligent materials. *J. Intell. Mater. Syst. Struct.*, **1990**, *1*, 149–156.
11. Mishr, A.K., Kavipriya J, Jose, E., Mohan, A., Akshay, M. Review study on smart nanomaterials and their applications. *Mater. Charact.,* **2022**, *1*(1), 32–42.
12. Drossel, W.G., Kunze, H., Bucht, A., Weisheit, L., Pagel, K. Smart^3-Smart materials for smart applications. *Procedia CIRP*, **2015**, *36*, 211–216.
13. Aflori, M. Smart nanomaterials for biomedical applications—a review. *Nanomaterials*, 2021, *11*, 396.
14. Damodharan, J., Sreedharan, A., Ramalingam, T. A review on smart materials, types and applications. *Int. J. Eng. Technol. Sci. Res.*, **2018,** *5*(3), 649–653.
15. Yoshida, M., Lahann, J. Smart nanomaterials. *Am. Chem. Soc.,* **2008**, *2*(6), 1101–1107.
16. Thompson, B.S., Gandhi, M.V., Kasiviswanathan, S. An introduction to smart materials and structures. *Mater. Design*, **1992,** *13*(1), 3–9.
17. Susmita, K. Introduction, classification and applications of smart materials: an overview. *Am. J. Appl. Sci.,* **2013,** *10*(8), 876–880.
18. Mrinalini, M., Prasanthkumar, S. Recent advances on stimuli-responsive smart materilass and their applications. *Chempluschem*, **2019**, *84*(8), 1103–1121, https://doi.org/10.1002/cplu.201900365.
19. Uma Maheswari, A., Lavanya, A., Vinay, E. Smart materials-types & applications. *Int. J. Res. Appl. Sci. Eng. Technol.*, **2022**, *10*(I), 1752–1755.
20. Spaggiari, A., Castagnetti, D., Golinelli, N., Dragoni, E., Scirè Mammano, G. Smart materials: properties, design and mechatronic applications. *J. Mater.*, **2016**, *0*(0), 1–29.
21. Levi, D.S., Kusnezov, N., Carman, G.P. Smart materials applications for pediatric cardiovascular devices. *Pediatr. Res.,* **2008**, *63*(5), 552–558.
22. Kumar Bohidar, S., Kumar, D., Ranjan Mishra, P., Sharma, R. Smart materials for future. *Int. J. Adv. Res. Sci. Eng.,* **2015**, *4*(2), 365–372.
23. Basheer, A.A. Advances in the smart materials applications in the aerospace industries. *Aircr. Eng. Aerosp. Technol.,* **2020,** *92*(7), 1027–1035.
24. Szolomicki, J. Application of smart materials in civil engineering and architecture. *IOP Conf. Series: Mater. Sci. Eng.,* **2020**, *958*, 012006.
25. Hamed, H.M.S. Smart material overview and their applications. *Int. J. Sci. Eng. Res.,* **2016**, *7*(8), 1413–1418.
26. Singh, M., Sharma, R.K., Singh, A.K., Prajapati, N. A study of smart materials, classification and applications: a review. *Int. J. Manag. Technol. Eng.,* **2018**, *8*(5), 165–169.

27. Rezaei, N., Akbarzadeh, I., Kazemi, S., Montazeri, L., Zarkesh, I., Hossein-Khannazer, N., Hassan, M., Vosough, M. Smart materials in regenerative medicine. *Mod. Med. Lab. J.*, **2021,** *4*(1), 39–51.
28. Cao, W., Cudney, H.H., Waser, R. Smart materials and structures. *Proc. Natl. Acad. Sci.*, **1999**, *96*, 8330–8331.
29. Aher, S.S., Desarda, A., Shelke, J.A., Chaudhari, M. A review on smart materials: future potentials in engineering. *Int. J. Sci. Technol. Manag.,* **2015**, *4*(10), 7–16.
30. Pandey, J., Solanki, P. Scope of smart materials in future. *Int. J. Eng. Res. Technol.*, **2021**, *10*(6), 26–37.
31. Wadhawan, V.K. Smart structures and materials. *Resonance*, **2005**, 27–41.
32. Nazem Qader, I., Kök, M., Dagdelen, F., Aydogdu, Y. A review of smart materials: researches and applications. *J. Sci. Eng.,* **2019**, *6*(3), 755–788.
33. Laws, J., Parachuru, R. New and emerging smart materials and their applications: a review. *J. Mater. Sci. Eng.*, **2021**, *10*, 1–6.

CHAPTER 4

GRAPHENE-BASED MATERIALS FOR SOLAR CELLS: REVIEW

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ABSTRACT

Graphene (GN) is unique by its two-dimensional (2D) structures which played a revolutionary role for conductive transparent devices and acquired an extraordinary possibility to be utilized in the energy sector. GN was combined with the photovoltaic (PV) concept in the last two decades, and has played an important role as interface layer in PV devices, charge carrier transport material, and thin transparent plates in PV systems. This chapter highlights many ways of graph production and the latest breakthroughs in graphic solar cells, including the organic, dyed-sensitive, and perovskite solar cell devices for bulk heterojunction. For GN perovskite PV cells, rate of energy conversion exceeded 20.3% and reached 10% for the organic PV device. GN has another special purpose in environmental protection through its specific large surface enhances not only sun exposure but also provides

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long-life stability for PV systems. It offers large charge carrier extraction and their easy transportation in between electrodes. A comparative research has emphasized on the function of GN and its products in solar systems. After all, the possible problems and prospects are provided for future graphic materials research for PV applications.

4.1 INTRODUCTION

Nonrenewable resources such as coal, petrol, etc. have a limited lifespan and cause worldwide environmental pollution. These energy sources harm our green planet and may result in catastrophe for mankind. Renewable sources are required to be uplifted as they are eco-friendly and act as a sustainable source of energy. Renewable energy sources could be preferred more. The great energy could be extracted from wind, sun, and water. They are providing clean, green, and very cheap energy and in the appropriate way, this energy transforms into electric energy. This generated energy is eco-friendly and pollution-free. Solar energy is not only cleanest but also available abundantly on the earth's surface. Solar energy could be renewed as electrical energy through photovoltaic (PV) setup. Utilizing the PV technique, solar radiation is directly converted into electric energy due to photoelectric effects. It is one of the cleanest forms of energy that is captured through solar cell systems installed in the direct sun. All solar cell consists of several components likewise broad panel, convertor, and storage devices. The transformation of photon energy into electric energy also depends on the material properties of the device. A variety of solar cells developed to achieve worthy efficiency. For enhancing durability, cost-effectiveness, and solar-to-electric conversion efficiency, solar cells are constantly undergoing modifications and updations. The efficiency of energy conversion through a solar cell depends upon the material used to develop the solar device. It was reported that, for significantly improved quality of PV parameters by different metal oxides, organic polymers, and semiconductors [1–4]. The semiconductor-based solar device is considered the first generation of a PV device. Matsui et al. [5] reported that with 11% efficiency Si-based PV devices capture the market. The thin-film solar cell effectively working the renewable energy source market, it is considered as the second generation of a solar cell. In the sequence of development of solar cells, dye sensitized solar cells, *quantum dot solar cell*, and organic photovoltaics are considered as the third generation of a PV device. The prevailing third-generation PV devices are more efficient, cost-effective, and eco-friendly. Recently, graphene (GN) has become a showstopper on the lime tight for such kinds of application devices. GN has an amazing electrical and optical property that is more suitable for household, small applications, and also commercial applications on a large scale. The history of GN is not so old, just two decades ago it was discovered by two scholars Andre Geim and Kostya Novoselov in 2004. Like carbon nanotube, fullerene, carbon black, etc., GN is one of the carbon allotropes. All allotropes of carbon are unique because of their properties, similarly, the unique properties of likewise GN have a unique structure that makes them special. High mechanical strength, zero bandgap, swift carrier mobility, and excellent thermal properties fascinated the attention of researchers to GN [6–9]. The use of GN as doping or main material shows many advantages for the various types of PV devices. The unique and amazing characteristics of GN are favorable for PV devices [10, 11]. The internal structure, mechanical property, thermal response, and electrical properties of GN provide the main advantage for introducing with any other organic, inorganic, metallic, or nonmetallic materials. Carbon allotropes can be also classified as 0D (fullerene), 2D (GN), and 3D (carbon nanotube) (Figure 4.1).

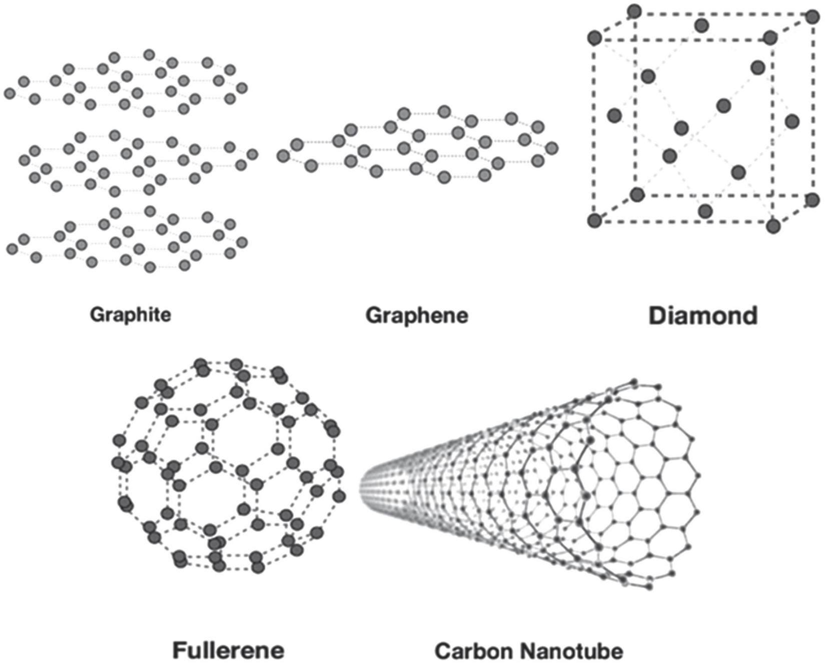


FIGURE 4.1 Allotropes of carbon. ⏎

In the last two decades, various derivatives of GN have been discovered. Reduced GN (r-GN) and graphene quantum dots (GQDs) are the most fascinating successor of GN [12]. GN and derivative of carbon have been depicted in Figure 4.2. The derivatives of GN have been obtained depending upon the synthesized techniques. In all the forms of GN, the major change occurs due to the functional groups that are attached in its basal plane and its edge. GN oxide is considered as the first derivate of graphite it is also known as graphitic acid. GO is decorated by various functionalities like carboxyl, epoxy, and hydroxyl groups as compared to other derivatives of GN [13–16]. These groups provide the large spacing between two consequent layers due to this interlayer spacing obtained almost twice of GN [15, 17]. This functionality enhances the strong reactivity and the solubility of nanomaterials in water and organic solvent. By specific techniques such as chemical processing, thermal processing these functionalities get eliminated, thus the final material is called reduced graphene oxide (rGO) [18]. The surface area of rGO also increases; it becomes more thermally conductive, chemically reactive, and stable. GQDs belong to the nanoparticle of GN but are considered a new class of material. GQDs have lateral dimensions ranging from 2 to 20 nm, which provides unique properties of photoluminescence (PL), high transparency, much sensitivity, and large surface area. It is a new hope for an excellent and fast display system [19–21].

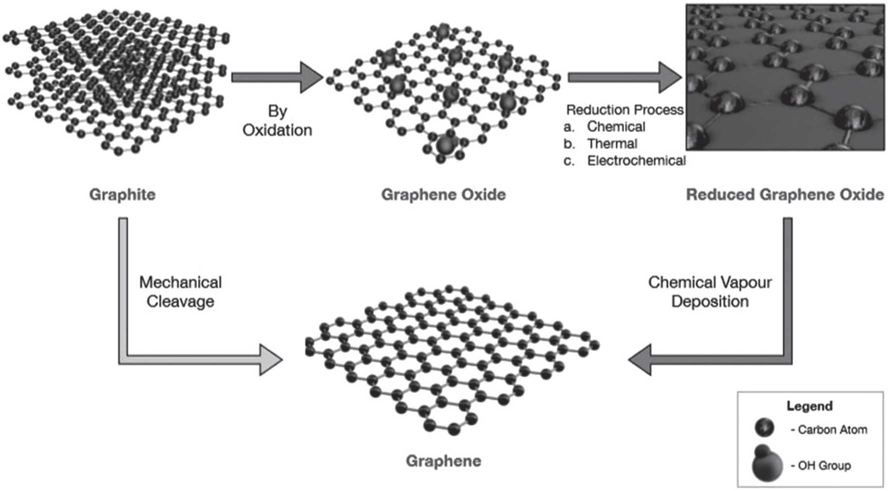

By
Oxidation
Reduction Process
a. Chemical
b. Thermal
c. Electrochemical
Graphite
Graphene Oxide
Reduced Graphene Oxide
Mechanical
Cleavage
Chemical Vapour
Deposition
Graphene
Legend
- Carbon Atom
- OH Group

FIGURE 4.2 Derivatives of GN. ⏎

GN has a 2D structure decorated with carbon atoms and looks like a honeycomb [22, 23]. The extraordinary basal plane of GN has an arrangement of sp^2 hybridized carbon atoms covalently [24]. The π bond becomes away from the plane and provides a free electron which is responsible for conduction [25]. GN is found in single or multilayer form. The width of the GN sheet is equal to the diameter of the carbon atom. Chemical vapor deposition (CVD) is a common technique for the synthesis of GN on metallic surfaces. Exceptional electrical conductivity, great charge mobility, high surface-to-volume ratio, optical response, and zero-structural defect give it uniqueness and make it an ideal nanomaterial [26, 27]. As per the surface, expanse GN has a large surface area as compared to other allotropes of carbon, it provides excellent interfacial interaction with other materials atom or matrix, during the fabrication of nanocomposites also. The large surface of GN inhibits or minimizes the cluster of atoms in nanocomposites [28, 29].

Functionalization plays a very important role to attain amazing properties and emerge various applications. Functional groups prevent the aggregation of atoms and increase the ability to disperse in any solvents [30–33]. During the oxidization process, these functional group molecules are attributed to the GN sheet either by adsorption (noncovalent bond) or by covalent bonds [34–37]. These functional groups enhance the processing ability of GN to implement significant purposes [38, 39]. In the case of durability or mechanical strength, GN presents a wonderful response. There are various research papers available that have been done on its mechanical characteristics like Young's modulus, elasticity, fracture strength, etc. The significance of mechanical properties is that devices are easily developed for numerous implementations in many fields. The fracture strength of 130 GPa of the monolayer GN sheet, and also it has Young's modulus of 1 TPa that shows the prepared film is defect-free [40]. The elastic modulus of GN strip without restraint suspended is 0.25 TPa [41]. Moreover, GN dispersion in inorganic nanomaterials enhanced the mechanical stability of synthesized GN-based nanocomposites [42].

Most researchers disclosed that GN has been reported as an excellent candidate for electrical conduction. It behaves like a semiconductor of zero bandgaps hence, at room temperature excessive electrons are transferred [43]. At room temperature, the reported value of charge mobility was 15000 $cm^2/V/s$ [44]. The charge carrier mobility increases tremendously by reducing the doping at the ambient condition that was observed at about 200,000 cm^2 /V/s [45]. Furthermore, it was also reported that in GN sheets the mobility of the charge carrier is free from the temperature [46]. Baladin et al. disclosed that the thermal response of monolayer GN was 5000 Watt/m/K by using the micro-Raman spectroscopy [47]. This thermal behavior is amazing for electronic applications, fuel cells, and batteries because this feature of GN provides thermal stability and work durability. GN shows a high optical conductive response. It was observed that many GN nanocomposites represent optical transparency [48, 49]. Mehmoudi et al. reported that GQDs, that is, zero-dimensional GN particles have quantum significance along with energy traps therefore, it provides excellent PL attribute [50]. The contribution of these optical characteristics in PV means like solar cells, advanced electronics, etc.

4.2 SELECTION OF MATERIALS AND SYNTHESIZED TECHNIQUES OF GN AND GN NANOCOMPOSITES

The fundamental properties of GN like morphology, interlayer separation, crystal size, electron mobility, thermal behavior, solubility, optical response, etc. all depend on synthesis technique. There are two techniques used for GN synthesis, one top-down technique and another bottom-up method. Through top-down technique, the graphite turns into GN oxide by chemical oxidization process or electrochemical exfoliation, in such technique during the oxidization, several oxygen function groups enter and are attached with GO plane, these functional groups could be replaced by thermal reduction [51]. Improved hummers method could be selected for this. The other technique of GN synthesis, that is, bottom-up started from gas molecules as a precursor. Physical vapor deposition (PVD), chemical vapor deposition (CVD), atomic layer deposition (ALD) techniques are commonly used for that [52–54]. Figure 4.3 shows different synthesis mechanisms of GN.

In the top-down technique, the obtained GN oxide is enriched with various oxygenated functionalities. By removing functionality, the GN is obtained in bulk, also this pure GN has different features [55–57]. The oxygen functionality could be eliminated by different techniques likewise thermodynamically and kinetically. With the heat treatment carboxyl and hydroxyl functionality is easily removed while epoxy functionality is eliminated by making use of hydrazine compound [58, 59]. The outcome of this reduction technique is called rGO, most obvious is the derivative of GO, which shows similar characteristics like GO, but during the reduction, the π-network re-established which improves the conductivity of the material.

In the bottom-up technique, the chemical vapor deposition process is generally used to produce pure, large-area, and high-performance GN.

In this technique, the GN layer is grown on the substratum of metallic or semiconductor wafers by the deposition of hydrocarbon vapor. There is a possibility that more than one gaseous vapor (precursors) decomposes on the metallic surface as the demand of the device. The substrate surface acts as a catalyst, when the precursor flows on the catalyst, it gets deposited, and a chemical reaction takes place. As per the purpose, the selected catalyst is either monomaterial or alloy of more than metal. The deficient d orbit metals promptly absorb and react with deposit carbon atom giving excellent performance. With the absorption of carbon atoms cobalt, copper and nickel subtract emerge polycrystalline GN material. The significance of these polycrystallines is their thermal stability [60].

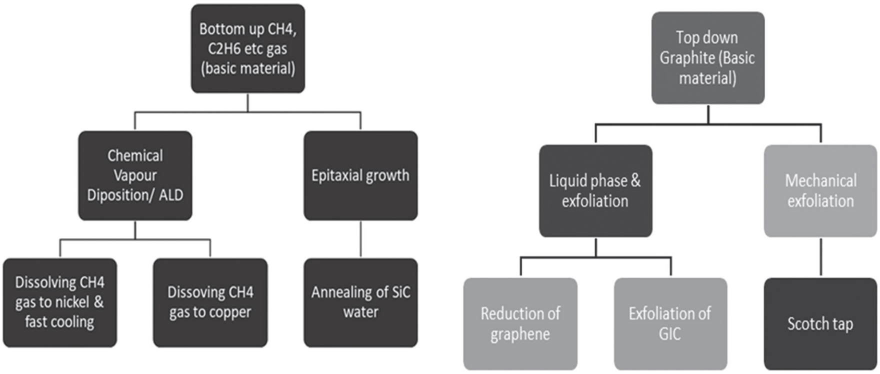

Bottom up CH4, C2H6 etc gas (basic material)
Chemical Vapour Diposition/ ALD
Epitaxial growth
Dissolving CH4 gas to nickel & fast cooling
Dissoving CH4 gas to copper
Annealing of SiC water
Top down Graphite (Basic material)
Liquid phase & exfoliation
Mechanical exfoliation
Reduction of graphene
Exfoliation of GIC
Scotch tap

FIGURE 4.3 Synthesis mechanism of graphene. ⏎

The size of the particle obtained by this technique is in nanosize but its range is about 10 to 20 nm. This size turns GN into GQDs. GQDs are a new member of the GN group which is considered a zero-dimensional particle. The reduction of size enhances the amazing properties of GN especially optical behavior and light emission. Zero-dimension particle size, effective bandgap, and optoelectronic properties give rise to significantly a better option for solar cells [61]. It is reported that biocompatibility, high sustainability, and nontoxicity properties are most useful for dye-sensitized solar cells (DSSCs) [62]. Recently, much research work has disclosed that the use of GN as quantum dot enhances the efficiency of transformation of solar radiation into electric power [63, 64]. The grown GN properties depend upon the flow of hydrocarbon gas vapor (precursor), the pressure of a gas, temperature, and the property of the surface of metallic material. It is mandatory that for the formation of GN structure aggregation of carbon molecules should be avoided. It was reported that by roll-to-roll production the 30-inch GN layer was deposit onto Cu wafer by CVD technique [65, 66].

4.3 EVALUATION OF GRAPHENE IN PHOTOVOLTAIC APPROACH

4.3.1 GN-ORGANIC SOLAR CELLS (OSCS)

In an organic solar cell, electrodes play a very important role, which are made by high conducting and optically transparent materials. Indium tin oxide is considered the best option for this. Stotter et al. reported that indium tin oxide offers 80% transparency in the industrial application, while on the glass coating, its resistivity is about 10–15 Ω/sq, which shows that the ITO is very appropriate for the PV system. Fluorine-doped tin oxide (FTO) is also the same candidate as ITO. But the major challenge with ITO is its cost. The indium is insufficient on the earth's surface, therefore lacking supply it becomes so costly that it is not more durable because of its brittle nature. Thus, there are various kinds of metal grids, organic, inorganic compounds, and oxides used as ITO alternative for the electrodes. But these materials have poor optical transparency [67–69]. The organic solar cell electrodes require materials that are not only flexible, durable, conductive, and thermal stable but high optical transparency properties. After the disclosure of GN properties, especially its optical response, it is used as an electrode of the organic solar cells [70–73]. In the comparative performance of different electrodes, GN is a material whose performance exceeds ITO as an electrode. GN is a far better material for both anode and cathode than ITO. Its wide surface area facilitates the high mobility of charge carriers along with high optical response, which makes GN a more accomplished material for the electrode [74-80].

It is observed that the GN properties depend on its preparation mechanism. CVD is one of the widely applied synthesis mechanisms of GN having an optical active nature. T is transmittance of PV devices, the value of T decreases with the increases in thickness of the GN sheet and its conductivity. Transmittance is reciprocal to the purity of material. In CVD, the transmittance of GN is poor as compared to hummer's method of synthesized GN [81, 82]. The comparative study of transmittance of various material-doped electrodes is represented in Table 4.1.

The GN synthesized by the CVD technique provides exceptional transparency and conductivity, as compared with Hummer's method. In CVD synthesis technique, the purity of GN is quite high. With large surface area and controlled number of layers, the multilayer GN syntheses can be possible with this technique. All these wonderful properties of synthesized GN played an excellent role in organic solar devices [83].

TABLE 4.1 Comparison Between GN-based TCE on the Basis of T and R ⏎

Graphene Source	T (%)	Rs (Ω/sq)	References
r-GO	79.9	1000	[90]
GN on Ni substrate	75.9	279	[91]
GN on Cu substrate	93	251	[92]
CVD (chemically modified)	91	31	[93]
Exfoliated-G	73	2400	[94]

Figure 4.4 depicts the evolution of GN on metallic surfaces. It is reported that the organic PV cells are generally fabricated through CVD GN electrodes. At the top layer, CVD GN is used due to its excellent transparency. Solar cells having a four-layered GN structure, good air sustainability, and high flexibility provide the efficiency of photo energy conversion about 3.2% with 90% transmittance of GN electrodes. This multilayered transparent CVD GN electrode provides a long-life work capability [84].

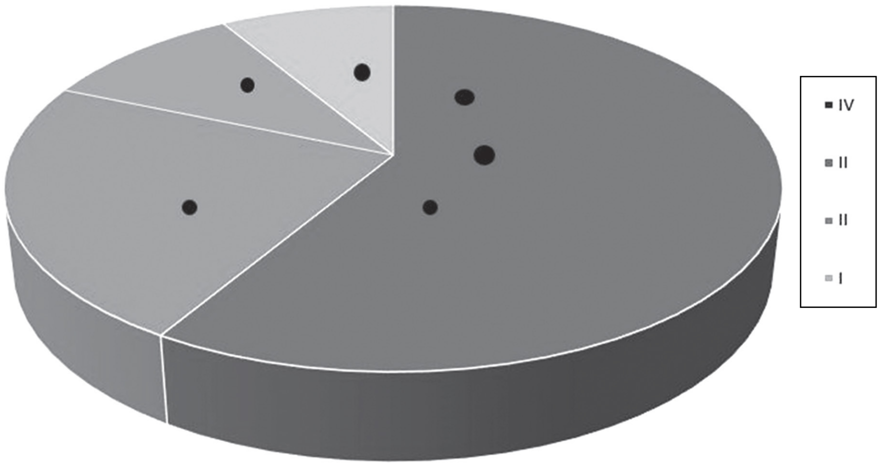


FIGURE 4.4 Graphene thin grow on a metallic surface by CVD technique (I) shows precursor (II) represents absorption of carbon atoms, (III) denotes segregation (IV) denotes catalytic process. ⏎

Table 4.2 represents evaluation of different material electrodes with respect to their characteristics. Since transmittance (T) of GN is reciprocal of their thickness of layer and conductivity (σ). Li et al. reported the comparison of T in between single and multilayer GN samples as compared to monolayer GN and multilayer GN. He disclosed that multilayered GN is more superior on the basis of conductivity, low transmittance, and higher air stability. The liquid exfoliation is preferred to synthesize the monolayer and multilayer GN, with increasing the layer the transparency of electrode obtained 93%, 88%, and 83%, respectively. This obtained value showed that transparency decreases with an increment of resistance [85].

The resistivity and transmittance are parameters associated with 2D conductivity σ2D and σo optical conductivity. However, conductivity depends on the GN properties or the synthesis technique of GN. The transmittance can be formulated as

$$T = [1 + (Z_0 /2R_s)(\sigma_0 /\sigma 2D)]{-}2 \tag{4.1}$$

where Z_0 represents the impedance of space, σo is clear that the transmittance is proportional to impedance, R_s is the resistance of electrode sheet which is proportional to the transparency of the electrode, σ_0 is present optical conductivity, while the optical conductivity of two-dimension $\sigma 2D$. The important outcome is reported that the resistance of electrodes depends upon the number of layers [86, 87]. The chemical doping enhances the conductivity of GN incorporated substrate therefore this technique transformed potentially semimetallic GN into metallic GN [88, 89]. Table 4.1 represents comparative study of diverse types of GN transparent conductive electrodes (TCE).

4.3.2 GN AS CHARGE ACCEPTOR SOLAR CELL

The inorganic solar cell materials should have the property by which they absorb solar radiation and enhance the capability and transform the solar radiation into potential as the band structure of materials plays a significant role. For the excellent performance, it should be necessary that the energy levels of the donor and acceptor materials must be aligned. In recipient and donor materials, the potential must be about 0.3 eV. To achieve good absorption of solar energy, the band gap of donor element should not be higher than 1.5 eV (102). The 2D structure of GN is always supported as a receiver and its fast charge transfer property is more compatible as well as suitable for donor candidates. This property shows excellent coordination of the energy bandgap [103, 104]. GN is a basic building block element

TABLE 4.2 Evaluation of Basic Parameters of Electrodes Fabricated by Different Materials

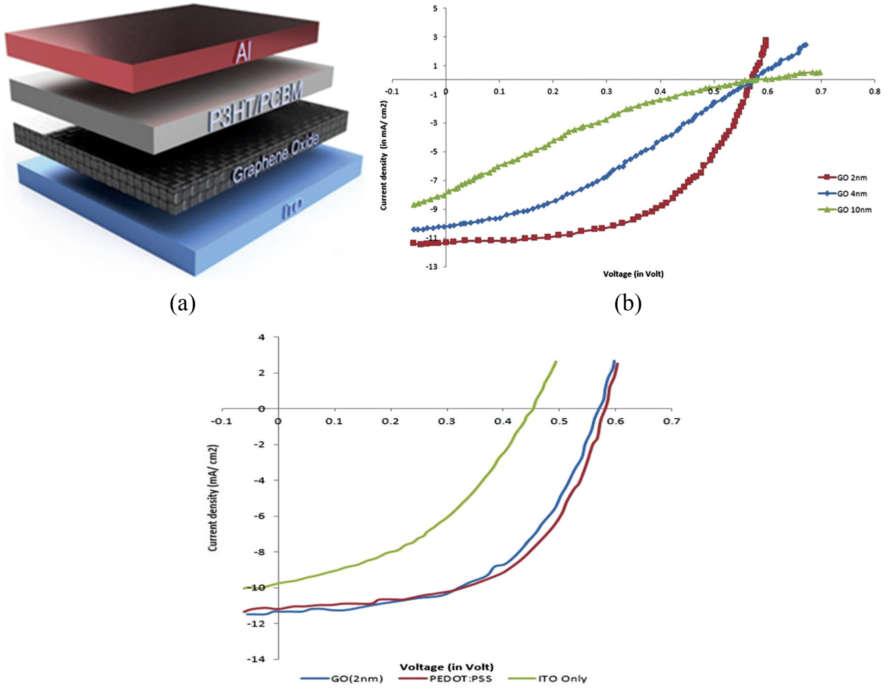
Materials	Transmittance (%)	Resistance (Ω/sq)	Color	Flexibility	Chemical stability	Haze	Drawback	Refs.
GN	>90	100–400	Colorless	Good	Excellent	Less	Less sensitive Low defect and impurity	[95,96]
Metallic nanoparticles	89	1–151	Colorless	Normal	Normal	Large	Need sintering	[97]
Organic materials	90	150	Colorless	Good	Good	Average		[98]
ITO	91	~19,000	Slightly yellow	Less	Normal	Less	Brittle, Costly	[101]

in which several allotropes of carbon can be built. Fullerene is one of the examples of such molecules. The fast charge receiving property distinguishes it from the rest of the materials. With the help of this property, the OSCs could be modified. Cho et al. observed that the PCBM (phenyl-C61-butyric acid methyl ester) was implemented for the modification of SOCs [105]. The introduction of GN in such ways reveals a superior combination with donner candidate because of their morphological and chemical properties. It was reported that the combination of GN as a recipient candidate with poly (3-dodecylthiophene) and poly(3-hexylthiophene) [106]. The outcomes of this experiment were amazing, the absorbance occurred in the range of 350–650 nm of wavelength while the PL emission was obtained between 600 and 800 nm. The combination of poly(3-octylthiophene) with GN performed a superb PV effect. It was reported that the electrons and holes were transmitted through the material structure, for the excellent transition it is necessary to select those materials which have the highest occupied molecular orbit or LUMO levels [102]. It was reported that the thin film of GO exhibits electron blockers and great positive charge transport in OSCs. Shao et al. fabricated a PV device by the use of photoactive poly (3-hexylthiophene) (P3HT):phenyl-C61-butyric acid methyl ester (PCBM) layer in between GO layer by synthesis of neural solution. In Figure 4.5(a), the first layer is synthesized by ITO which is highly conductive and transparent to provide fast transmission of radiation and reduces the leakage current and recombination of electrons with holes. The result of GO layer arrangement as hole transport layer enhances the OSC's efficiency compared to conventional hole transport layer OSCs, synthesis with PEDOT: PSS as the positive carrier conduction layer [103].

4.3.3 GRAPHENE AS AN ELECTRON-TRANSPORT LAYER (ETL)

In PV cells, the main role is played by the cathode electrode for extracting and collecting the charge carriers. The selection of the interface material should be more efficient and sustainable for the production of electric energy. The electron transport layer provides all the solutions by enhancing the efficiency parameters [90]. It should be also necessary that the synthesis electron extraction material film is thin so that the electrons are easily transferred toward lithium fluoride [104], conjugated polymer electrolytes [105], TiO_2, TiOx film as n-type semiconductors, GN as an electrode for dye-sensitized SC's ZnO [106, 107], n-type organic semiconductors [108] are used as electron carrier layer included in the PV device. It is also reported that GN as an electrode for dye-sensitized SCs using ZnO enhances 36% performance of solar cells [109].

It was reported that the synthesis of GN thin layer approx 1 nm thickness, if it directly introduces as negative carrier transport layer in the middle of bulk heterojunction (BHJ), an electrode in ITO/PEDOT:PSS/PCDTBT:PC71BM/GO/Al that enhance the significate outcome of solar device likewise ~7% improvement in PCE [110]. The PCE of such PV cells is enhanced up to 6.72% with FF = 64% and revised value in J_{sc}=13 mA/cm^2 while the PV device fabricated without GN electron transport layer the PCE is 5.35%, FF= 58%, and J_{sc}= 10.66 mA/cm^2. It is also reported that using GN-based ETL the stability improved, in the terms of PCE decrement with GN-based ETL it is about 3% while without GN ETL the decrement percentage of PCE is about 56% obtained in the same manner TiO or GN-coated substrate, GO/TiOx electron transport film exhibits the maximum PCE of ~8% (Figure 4.6 a and b).



(a)

(b)

(c)

FIGURE 4.5 (a) Demonstration of ITO/GO/P3HT:PCBM/Al photovoltaic device; (b) I–V curve OSCs with no hole transport layer; (c) I–V curve of ITO/GO/P3HT: PCBM/Al combination in various width of GO film. ⏎

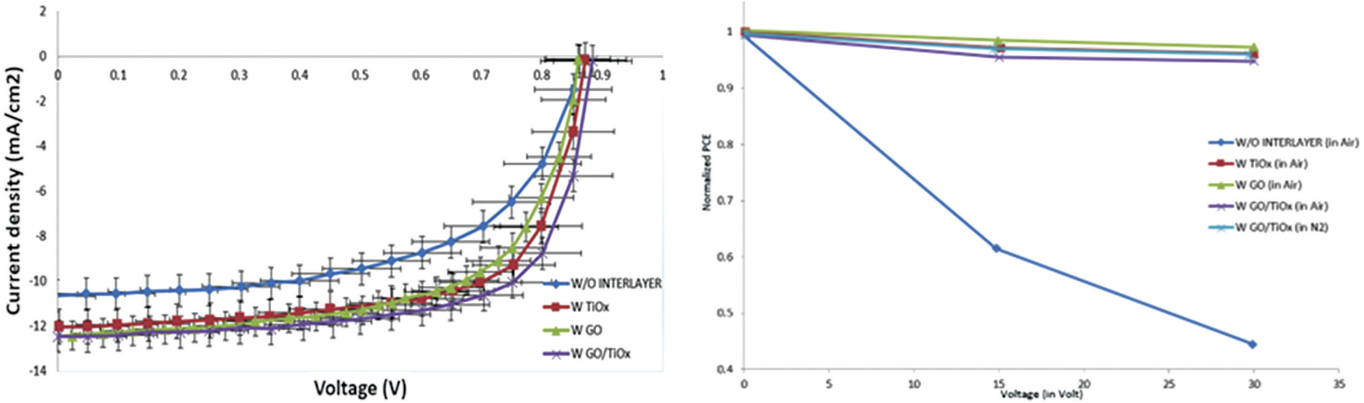


FIGURE 4.6 (a) Current density–V curve of BHJ with and without an ETL layer of TiOx, GO, and GO/TiOx; (b) PCE vs voltage graphene as an electrode in DSSCs. ⏎

FTO is a highly transparent metal oxide material that is used in the preparation of transparent electrodes for PVs like an organic PVs, dye-DSSCs, and hybrid perovskites. The implementation of silicon solar cells becomes costly on large scale. The dye-sensitized cell is a wonderful replacement for silicon solar cells and also by DSSC obtained better results compared to conventional semiconductors after the invention of the DSSC [111, 112]. This combination provides a large porous surface which gives excellent performance after the emergence of molecular sensitizer solution or photosensitive dye solution with the combination of Pt platinum material plate on which iodide electrolyte spread and both are combined. Normally, to prevent the leakage of electrolytes, the solution vessel is sealed.

DSSC based on photogeneration of an electron by the dye works differently from conventional SCs. In DSSC, photoexcitation of the sensitizer dye results in the incorporated electrons into the TiO_2 surface [115]. To obtain extraordinary performance, GN could be used in each part of the dye. The oxygen functional group's accomplishment is vigorous in catalytic reactions. The redox chemical effect of electrolyte GN is more favorable compared to platinum electrodes. As compared to pure GN, doped GN performed as counter electrodes in a much better way [116, 117] along with that, the scaffold shape of 3D GN is good for counter electrodes [118]. It was reported that in dye solar cells PCE is enhanced by using rGO because of its high charge mobility [119].

4.3.4 GN-PEROVSKITE SOLAR CELLS (PSCs)

Perovskite materials are cost-effective and greatly efficient for the preparation of solar cells [120]. Kojima et al. reported that the first time the $CH_3NH_3PbX_3$ perovskite organo-lade halide materials where (X=Br, I) were used in DSSCs. In the beginning, with the use of inorganic materials like bromine (Br) or iodine (I), the value of power conversion efficiency was enhanced by 3.8% or 3.1%, respectively [121]. By some change in material selection and also the synthesis technique of the perovskite layer the recombination of electrons decreases, which enhances its PCE value on an average of 16.6% [122]. Starnks et al. reported that in the analysis of various parameters like a lifetime, carrier diffusion length, etc. of triiodide $CH_3NH_3PbI_3$ and mixed halide $CH_3NH_3PbI_3$-xClx pervoskite layer, the result shows that the diffusion length of $CH_3NH_3PbI_3$-xClx is larger than 1, high carrier mobility and large absorption coefficient that improve PCE performance and enhance the stability of the SCs [123–126]. Liang et al. reported that due to additives materials and preparation techniques of film on the substrate have high impact in perovskite surface, which facilitates high PCE about 12% [127]. The metal oxide required of high temperature for charge transferring processing. The basic structure of the PSCs is similar to DSSCs, both devices require high threshold temperatures for their working. That is the biggest challenge for initiating the process [128–131]. Liu et al. disclosed that by the adoption of triple material Sphenyl-C61-butyric acid methyl ester (PCBM), C60, and LiF layers cathode buffer as a component in perovskites solar cell. In such devices, PEDOT:PSS is arranged as electron–hole transporter. The thin LiF film promotes the carrier collection process that improves PCE of PSCs up to 15% [132–138].

To design PSCs by using a simple chemical approach with a reduced-graphene scaffold (rGS) that offers a high surface area. In perovskite solar cell rGS layer is developed in between charge absorber and charge transport layer. The hollow structure of GN and 3D are two properties enhanced scaffold of the large surface area of GN developed using electrophoretic techniques. The use of rGS enhanced 17.2% PCE of pervoskite solar cell. The value of J_{sc} = 23 mA/cm^2, V_{oc} =1.06 V, and fill factor = 72%. Figure 4.7 depicts the comparative curve between PSCs and TiO$_2$ device [139].

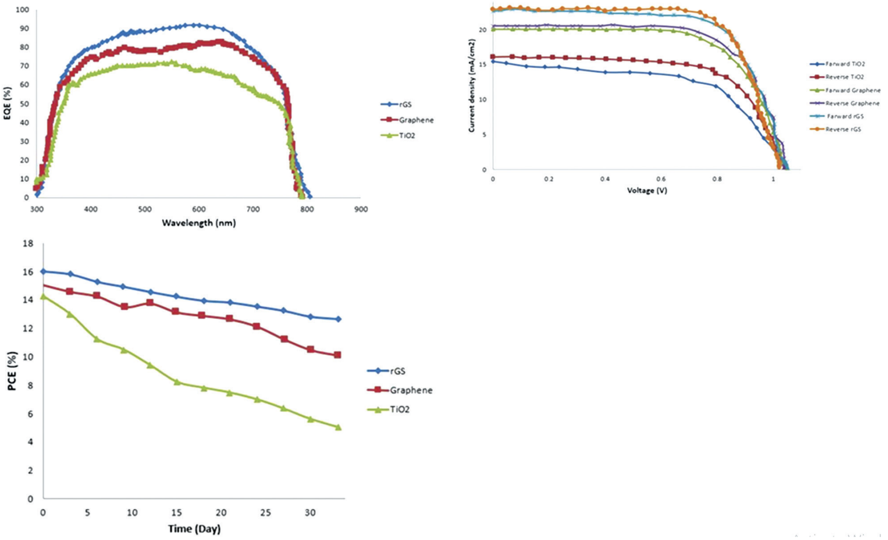


FIGURE 4.7 (a) EQE vs. wavelength spectra, (b) J−V curve (c) Stability curve between time and PCE. ⏎

4.4 CONCLUSION

In this chapter, we review how to enhance green energy with GN. Extraordinary properties of GN-like zero bandgaps, high carrier mobility, optical response, and mechanical and thermal properties uplifted it, compared to conventional materials. By introducing GN, the PV effect remarkably changes. These changes take place only when the GN is synthesized for a particular purpose, which is also very compatible with complementary materials. The synthesized methodology plays a vital role in establishing the significant properties in the GN, by which the various potential applications are executed. Few facile, adaptable, and suitable synthesis techniques are discussed in this chapter. The most suitable synthesis technique is chosen for GN manufacturing depending upon its application area. Likewise, the thermal reduction technique is excellent for rGO preparation. The rGO attributes great compatibility with conductive polymers, conducting compounds, and conducting metallic oxides, these enhance the conductivity of GN-based nanocomposite or sheet. The GN-incorporated conducting polymer not only enhances the conductivity but also attributes flexibility. The performance of electrodes fabricated by such material is highly compatible with TCEs accomplishment. These types of electrodes represent a promising application; organic solar cell is a simple example of it. The other main fascinating reason to use GN in a solar cell is its large surface area and honeycomb structure, which provides more stability against the change in the atmosphere. Therefore, with a smart selection of complementary compound with GN, all those problems have been resolved which are common for conventional solar cells. Although GNs have wonderful properties and hold promising potential for contributions to green energy system, synthesizing GN in bulk remains one of the biggest challenges. Another challenge is the installation of these solar systems for commercial purposes in a cost-effective manner, although household or small devices, such as solar geysers and solar calculators, can be easily managed. It should be necessary to emerge GN-based PV applications purposefully. The outstanding conductivity, eco-friendly nature, high flexibility, and compatible production approach make GN a world-class material for green energy resources. Now it is time to revolutionize the conventional solar system with GN with appropriate technology.

KEYWORDS

- **graphene**
- **metallic nanoparticles**
- **organic solar cell**
- **carrier conductive layer**

REFERENCES

1. Miao, X., Tongay, S., Petterson, M.K., Berke, K., Rinzler, A.G., Appleton, B.E., Hebard, A.F. *Nano Lett.*, **2012**, *12,* 2745.
2. Shi, E., Li, H., Yang, I., Zhang, I., Li, Z., Li, P., Shang, Y., Wu, S., Li, X., Wei, J., Wang, K., Zhu, H., Wu, D., Fang, Y., Cao, A. *Nano Lett.*, **2013**, *13,* 1776.
3. Song, Y., Li, X., Mackin, C., Zhang, X., Fang, W., Palacios, T., Zhu, H., Kong, J. *Nano Lett.,* **2015**, *15,* 2104.
4. Bhopal, M.F., Lee, D.W., Rehman, A.U., Lee, S.H. *J. Mater. Chem., C.,* **2017**, *5*, 10701.
5. Matsui, T., Sai, H., Suezaki, T., Matsumoto, M., Saito, K., Yoshida, I., Kondo, M. In *European Photovoltaic Solar Energy Conference & Exhibitio,* 2013, pp. 2213–2217.
6. Zhu, Y., James, D.K., Tour, J.M. *Adv. Mater.,* **2012**, *24,* 4924.
7. Zhan, D., Yan, J.X., Lai, L.F., Ni, Z.H., Liu, L., Shen, Z.X. *Adv. Mater.,* **2012**, *24,* 4055.
8. Huang, X., Qi, X.Y., Boey, F., Zhang, H. *Chem. Soc. Rev.,* **2012**, *41,* 666.
9. He, Q., Wu, S., Yin, Z., Zhang, H. *Chem. Sci.,* **2012,** *3*, 1764.
10. Thoteson, E.T., Ren, Z.F., Chou, T.W. *Compos. Sci. Technol.,* **2001**, *61,* 1899–1912.
11. Qian, H., Greenhalgh, E.S., Shaffe, M.S.P., Bismarck, A. *J. Mater. Chem.,* **2010**, *20,* 4751–4762.
12. Peña-Bahamonde, J., Nguyen, H.N., Fanourakis, S.K., Rodrigues, D.F. *J. Nanobiotechnol.,* **2018**, *16,* 1–17.
13. Xu, L., Wen, Y., Pandit, S., Mokkapati, V.R.S.S., Mijakovic, I., Li, Y. *BMC Chem.,* **2019**, *13,* 1–12.
14. Sharma, D., Kanchi, S., Sabela, M.I., Bisetty, K. *Arab. J. Chem.* **2016**, *9*, 238–261.
15. Talyzin, A.V., Solozhenko, V.L., Kurakevych, O.O., Szabo, T., Dekany, I., Kurnosov, A. *Chem. Int. Ed.,* **2008**, *47,* 8268–8271.
16. Krishnan, D., Kim, F., Luo, J., Cruz-Silva, R., Cote, L.J., Jang, H.D. *Nano Today,* **2012**, *7*, 137–152.
17. Rao, C.N.R., Sood, A.K., Subrahmanyam, K.S., Govindaraj, A. *Angew. Chem. Int. Ed.,* **2009**, *48,* 7752–7777.
18. Papageorgiou, D.G., Kinloch, I.A., Young, R.J. *Carbon,* **2015**, *95,* 460–484.
19. Zhang, Z., Zhang, J., Chen, N., Qu, L. *Energy Environ. Sci.,* **2012**, *5*, 8869–8890.
20. Shen, J., Zhu, Y., Yang, X., Li, C. *Chem. Commun.* **2012,** *48*, 3686–3699.
21. Elvati, P., Baumeister, E., Violi, A. *RSC Adv.,* **2017,** *7*, 17704–17710.
22. Netharavati, C., Rajamathi, M., Ravishankar, N., Basit, L., Felser, C. *Carbon,* **2010**, *48,* 4343–4350.

23. Jiang, B.J., Tian, C.G., Zhou, W., Wang, J.Q., Xie, Y., Pan, Q.J., Ren, Z.Y. Dong, Y.Z., Fu, D., Han, J.L., Fu, H.G. *Chem. Eur. J.,* **2011**, *17,* 8379–8387.
24. Zhou, K.F., Zhu, Y.H., Yang, X.L., Li, C.Z. *New J. Chem.,* **2010**, *34,* 2940–2955.
25. Leenaerts, O., Peelaers, H., Hernández-Nieves, A., Partoens, B., Peeters, F. *Phys. Rev. B,* **2010**, *82,* 195436.
26. Arun, T., Verma, S.K., Panda, P.K., Joseyphus, R.J., Jha, E., Akbari-Fakhrabadi, A. *Mater. Sci. Eng. C,* **2019**, *104,* 109932.
27. De, S., Mohanty, S., Nayak, S.K., Verma, S.K., Suar, M. *Nano,* **2015**, *10,* 1550091.
28. Jin, Z., Nackashi, D., Lu, W., Kittrell, C., Tour, J.M. *Chem. Mater.,* **2010**, *22,* 5695–5699.
29. Stankovich, S., Dikin, D.A., Pine, R.D., Kohlhaas, K.L., Kleinhmmers, A., Jia, Y., Wu, Y., Nguyen, S.T., Ruoff, R.S. *Carbon,*, **2007**, *45,* 1558–1565.
30. Niyogi, S., Bekyarova, E., Itkis, M.E., McWilliams, J.L., Hamon, M.A., Haddon, R.C. *J. Am. Chem. Soc.*, **2006**, *128,* 7720-7721.
31. Xu, Y.X., Bai, H., Lu, G.W., Li, C., Shi, G.Q. *J. Am. Chem. Soc.,* **2008**, *130,* 5856–5857.
32. Quintana, M., Spyrou, K., Grzelczak, M., Browne, W.R., Rudolf, P., Prato, M. *ACS Nano.*, **2008**, *4*, 3527–3533.
33. Ramanathan, T., Abdala, A.A., Stankovich, S., Dikin, D.A., Herrera-Alonso, M., Piner, R.D., Adamson, D.H., Schniepp, H.C., Chen, X., Ruoff, R.S., Nguyen, S.T., Aksay, I.A., Prud'homme, R.K., Brinson, L.C. *Nat. Nanotechnol.,* **2008**, 327–331.
34. Patil, A.J., Vickery, J.L. Scott, T.B., Mann, S. *Adv. Mater.,* **2009**, *21,* 3159–3164.
35. Liang, Y.Y., Wu, D.Q., Feng, X.L., Mullen, K. *Adv. Mater.,* **2009,** *21,* 1679–1683.
36. Yang, H.F., Shan, C.S., Li, F.H., Han, D.X., Zhang, Q.X., Niu, L. *Chem. Commun.,* **2009,** 3880–3882.
37. Hsiaso, M.C., Liao, S.H., Yen, M.Y., Liu, P.I., Pu, N.W., Wang, C.A., Ma, C.C.M. *ACS Appl. Mater. Interfaces.,* **2010**, *2*, 3092–3099.
38. Liu, Z.F., Liu, Q., Huang, Y., Ma, Y.F., Yin, S.G., Zhang, X.Y., Sun, W., Chen, Y.S. *Adv. Mater.,* **2008**, *20,* 3924–3930,
39. Li, X.L., Wang, X.R., Zhang, L., Lee, S.W., Dai, H.J *Science*, **2008,** *319,* 1229–1232.
40. Tung, V.C., Chen, L.M., Allen, M.J., Wassei, J.K., Nelson, K., Kaner, R.B., Yang, Y. *Nano Lett*., **2009**, *9*, 1949–1955.
41. Gomez-Navrro, C., Burghard, M., Kern, K. *Nano Lett*., **2008**, *8*, 2045–2049.
42. Jeon, K.J., Lee, Z. *Chem. Commun.,* **2011,** *47,* 3610–3612.
43. Morozov, S.V., Novoselov, K.S., Katsnelson, M.I., Schedin, F., Elias, D.C., Jazczak, J.A., Geim, A.K. *Phys. Rev. Lett.,* **2008,** *100,* 016602.
44. Novoselov, K.S., Geim, A.K., Morozov, S.V., Jiang, D., Zhang, Y., Dubonos, S.V., Grigorieva, I.V., Firsov, A.A. *Science*, **2004**, *306,* 666–669.
45. Bolotin, K.I., Sikes, K.J., Jiang, Z., Klima, M., Fudenberg, G., Hone, J., Kim, P., Stomer, H.L. *Solid State Commun*. **2008,** *146*, 351–355.
46. Balandin, A.A., Ghosh, S., Bao I.Calizo, W.Z., Teweldebrhan, D., Miao, F., Lau, C.N. *Nano Lett*. **2008**, *8*, 902–907.
47. Hong, T.K., Lee, D.W., Choi, H.J., Shin, H.S., Kim, B.S. *ACS Nano.*, **2010**, *4*, 3861–3868.
48. Mahmoudi, T., Wang, Y., Hahn, Y.B. *Nano Energy,* **2018**, *47,* 51–65.
49. Swager, T.M. *ACS Macro Lett*., **2011**, *1*, 3–5.
50. Eswaraiah, V., Aravind, S.S.J., Ramaprabhu, S. *J. Mater. Chem.,* **2011**, 21.
51. Mijatovic, D., Eijkel, J., Van Den Berg, A. *Lab Chip,* **2005**, *5*, 492–500.
52. Cai, J., Ruffieux, P., Jaafar, R., Bieri, M., Braun, T., Blankenburg, S., Muoth, M., Seitsonen, A.P., Saleh, M., Feng, X. *Nature,* **2010**, *466,* 470–473.

53. Huh, S.H. *Thermal Reduction of Graphene Oxide*. INTECH Open Access Publisher, 2011.
54. Chen, W., Yan, L., Bangal, P.R. *Carbon,* **2010**, *48,* 1146–1152.
55. Park, S., An, J., Potts, J.R., Velamakanni, A., Murali, S., Ruoff, R.S. *Carbon,* **2011**, *49,* 3019–3023.
56. Gao, X., Jang, J., Nagase, S. *J. Phys. Chem. C,* **2009**, *114,* 832–842.
57. Mahmoudi, T., Rho, W.-Y., Yang, H.-Y., Silva, S.R.P., Hahn, Y.-B. *Chem. Commun.,* **2014**, *50,* 8705–8708.
58. Muñoz, R., Gómez-Aleixandre, C, *Chem. Vap. Depos.,* **2013**, *19,* 297–322.
59. Bacon, M., Bradley, S.J., Nann, T. *Part. Part. Syst. Char.,* **2014**, *31,* 415.
60. Sharma, D., Jha, R., Kumar, S. *Sol. Energy Mater. Sol. Cells,* **2016**, *155*, 294.
61. Wang, H., Sun, P., Cong, S., Wu, J., Gao, L., Wang, Y., Dai, X., Yi, Q., Zou, G. *Nanoscale Res. Lett.,* **2016**, *11,* 27.
62. Feng, J., Dong, H., Pang, B., Shao, F., Zhang, C., Yu, L., Dong, L. *Phys. Chem. Chem. Phys.,* **2018**, *20,* 15244.
63. Kumar, S., McEvoy, N., Kim, H.Y., Lee, K., Peltekis, N., Rezvani, E., Nolan, H., Weidlich, A., Daly, R., Duesberg, G.S. *Phys. Status Solidi* (b), **2011**, *248*, 2604–2608.
64. Bonaccorso, F., Sun, Z., Hasan, T., Ferrari, A. *Nat. Photon.,* **2010**, *4*, 611–622.
65. Park, J.-H., Kang, S.J., Na, S.-I., Lee, H.H., Kim, S.-W., Hosono, H., Kim, H.-K. *Sol. Energy Mater. Sol. Cells,* **2011**, *95,* 2178–2185.
66. Choi, Y.-Y., Choi, K.-H., Lee, H., Lee, H., Kang, J.-W., Kim, H.-K. *Sol. Energy Mater. Sol. Cells,* **2011**, *95,* 1615–1623.
67. Park, J.-H., Ahn, K.-J., Na, S.-I., Kim, H.-K. *Sol. Energy Mater. Sol. Cells,* **2011**, *95,* 657–663.
68. Yan, K., Fu, L., Peng, H., Liu, Z. *Acc. Chem. Res.,* **2013**, *46,* 2263–2274.
69. Bae, S., Kim, H., Lee, Y., Xu, X., Park, J.-S., Zheng, Y., Balakrishnan, J., Lei, T., Kim, H.R., Song, Y.I. *Nat. Nanotechnol.,* **2010**, *5*, 574–578.
70. Yin, Z., Wu, S., Zhou, X., Huang, X., Zhang, Q., Boey, F., Zhang, H. *Small,* **2010**, *6,* 307–312.
71. Park, H., Chang, S., Zhou, X., Kong, J., Palacios, T.S., Gradečak, S. *Nano Lett*., **2014**, *14*, 5148–5154.
72. Zhang, D., Choy, W.C., Wang, C.C., Li, X., Fan, L., Wang, K., Zhu, H. *Appl. Phys. Lett.* **2011**, *99,* 259.
73. Lee, B.H., Lee, J.H., Kahng, Y.H., Kim, N., Kim, Y.J., Lee, J., Lee, T., Lee, K. *Adv. Funct. Mater.,* **2014**, *24,* 1847–1856.
74. Park, H., Chang, S., Zhou, X., Kong, J., Palacios, T., Gradecak, S., *ECS Trans*., **2015**, *69,* 77–82.
75. Yin, Z., Zhu, J., He, Q., Cao, X., Tan, C., Chen, H., Yan, Q., Zhang, H. *Adv. Energy Mater.,* **2014**, *4*.
76. Khrapach, I., Withers, F., Bointon, T.H., Polyushkin, D.K., Barnes, W.L., Russo, S., Craciun, M.F. *Adv. Mater.,* **2012**, *24,* 2844–2849.
77. Koh, W.S., Gan, C.H., Phua, W.K., Akimov, Y.A., Bai, P. *IEEE J. Sel. Top. Quantum Electron.,* **2014**, *20,* 36–42.
78. Bin Mohd Yusoff, A.R., Kim, D., Schneider, F.K., da Silva, W.J., Jang, J. *Energy Environ. Sci.,* **2015**, *8*, 1523–1537.
79. Cai, W., Zhu, Y., Li, X., Piner, R.D., Ruoff, R.S. *Appl. Phys. Lett.,* **2009**, *95,* 123115.
80. Petridis, C., Konios, D., Stylianakis, M.M., Kakavelakis, G., Sygletou, M., Savva, K., Tzourmpakis, P., Krassas, M., Vaenas, N., Stratakis, E., Horiz, N. **2016**, *1*, 375–382.
81. Gómez-Navarro, C., Meyer, J.C., Sundaram, R.S., Chuvilin, A., Kurasch, S., Burghard, M., Kern, K., Kaiser, U. *Nano Lett*. **2010**, *10,* 1144–1148.

82. Wang, X., Zhi, L., Tsao, N., Tomović, Ž., Li, J., Müllen, K. *Angew. Chem.* **2008**, *120,* 3032–3034.
83. Wang, Y., Tong, S.W., Xu, X.F., Özyilmaz, B., Loh, K.P. *Adv. Mater.,* **2011**, *23,* 1514–1518.
84. Liu, Z., Li, J., Yan, F. *Adv. Mater.* **2013**, *25,* 4296–4301.
85. Li, X., Zhang, G., Bai, X., Sun, X., Wang, X., Wang, E., Dai, H. *Nat. Nanotechnol.* **2008**, *3* 538–542.
86. Sun, Y., Zhang, W., Chi, H., Liu, Y., Hou, C.L., Fang, D. *Renew. Sustain. Energy Rev.,* **2015**, *43,* 973–980.
87. Han, X., Chen, Y., Zhu, H., Preston, C., Wan, J., Fang, Z., Hu, L. *Nanotechnology,* **2013**, *24,* 205304.
88. Romero, H.E., Shen, N., Joshi, P., Gutierrez, H.R., Tadigadapa, S.A., Sofo, J.O. Eklund, P.C. *ACS Nano,* **2008**, *2*, 2037–2044.
89. Shim, J., Lui, C.H., Ko, T.Y., Yu, Y.-J., Kim, P., Heinz, T.F., Ryu, S. *Nano Lett*., **2012**, *12,* 648–654.
90. Stankovich, S., Dikin, D.A., Dommett, G.H., Kohlhaas, K.M., Zimney, E.J., Stach, E.A., Piner, R.D., Nguyen, S.T., Ruoff, R.S. *Nature,* **2006**, *442,* 282–286.
91. Wang, Y., Chen, X., Zhong, Y., Zhu, F., Loh, K.P. *Appl. Phys. Lett.,* **2009**, *95,* 063302.
92. Park, H., Brown, P.R., Bulović, V., Kong, J. *Nano Lett*., **2011**, *12,* 133–140.
93. Parvez, K., Li, R., Puniredd, S.R., Hernandez, Y., Hinkel, F., Wang, S., Feng, X., Müllen, K., *ACS Nano,* **2013**, *7*, 3598–3606.
94. Wang, X., Zhi, L., Müllen, K. *Nano Lett*., **2008**, *8*, 323–327.
95. Wu, J., Becerril, H.A., Bao, Z., Liu, Z., Chen, Y., Peumans, P. *Appl. Phys. Lett.,* **2008**, *92,* 237.
96. Oyama, M. *Anal. Sci.,* **2010**, *26,* 1–12.
97. Shirota, Y. *J. Mater. Chem.,* **2000**, *10,* 1–25.
98. Charlier, J.-C., Blase, X., Roche, S. *Rev. Mod. Phys.,* **2007**, *79,* 677.
99. Ma, K., Yan, X., Guo, Y., Xiao, Y. *Eur. Phys. J. B-Condens. Matter Complex Syst.,* **2011**, *83,* 487–492.
100. Kim, H., Gilmore, C., Pique, A., Horwitz, J., Mattoussi, H., Murata, H., Kafafi, Z., Chrisey, D. *J. Appl. Phys.* **1999**, *86,* 6451–6461.
101. Bégué, D., Guille, E., Metz, S., Arnaud, M., Silva, H.S., Seck, M., Fayon, P., Dagron Lartigau, C., Iratcabal, P., Hiorns, R. *RSC Adv.,* **2016**, *6,* 13653–13656.
102. Liu, Z., Liu, Q., Huang, Y., Ma, Y., Yin, S., Zhang, X., Sun, W., Chen, Y. *Adv. Mater.,* **2008**, *20,* 3924–3930.
103. Mahmoudi, T., Seo, S., Yang, H.-Y., Rho, W.-Y., Wang, Y., Hahn, Y.-B. *Nano Energy.* **2016**, *28,* 179–187.
104. He, Z., Zhong, C., Huang, X., Wong, W.Y., Wu, H., Chen, L., Su, S., Cao, Y. *Adv. Mater.,* **2011**, *23,* 4636–4643.
105. Yip, H.L., Hau, S.K., Baek, N.S., Ma, H., Jen, A.K.Y. *Adv. Mater.,* **2008**, *20,* 2376–2382.
106. Kim, J.Y., Kim, S.H., Lee, H.H., Lee, K., Ma, W., Gong, X., Heeger, A.J. *Adv. Mater.,* **2006**, *18,* 572–576.
107. Chu, T.-Y., Lu, J., Beaupré, S., Zhang, Y., Pouliot, J.-R., Wakim, S., Zhou, J., Leclerc, M., Li, Z., Ding, J., *J. Am. Chem. Soc.,* **2011**, *133,* 4250–4253.
108. Lee, H.W., Oh, J.Y., Lee, T.I., Jang, W.S., Yoo, Y.B., Chae, S.S., Park, J.H., Myoung, J.M., Song, K.M., Baik, H.K. *Appl. Phys. Lett.,* **2013**, *102,* 193903.
109. Wang, D.H., Kim, J.K., Seo, J.H., Park, I., Hong, B.H., Park, J.H., Heeger, A.J. *Angew. Chem. Int. Ed.,* **2013**, *52,* 2874–2880.
110. Gabor, N.M., *ACC Chem. Res.* **2013**, *46,* 1348–1357.

111. Li, Y., Hu, Y., Zhao, Y., Shi, G., Deng, L., Hou, Y., Qu, L. *Adv. Mater.,* **2011**, *23,* 776–780.
112. O'regan, B., Grfitzeli, M. *Nature,* **1991**, *353,* 737–740.
113. Roy-Mayhew, J.D., Aksay, I.A. *Chem. Rev.,* **2014**, *114*, 6323–6348.
114. Cho, H.-H., Cho, C.-H., Kang, H., Yu, H., Oh, J.H., Kim, B.J. *Korean J. Chem. Eng.,* **2015**, *32,* 261–267.
115. Zheng, H., Neo, C.Y., Ouyang, J. *ACS Appl. Mater. Interfaces,* **2013**, *5*, 6657–6664.
116. Zhao, J., Wu, J., Zheng, M., Huo, J., Tu, Y. *Electrochim. Acta,* **2015**, *156*, 261–266.
117. Yang, N., Zhai, J., Wang, D., Chen, Y., Jiang, L. *ACS Nano,* **2010**, *4*, 887–894.
118. Neo, C.Y., Ouyang, J. *Carbon,* **2013**, *54,* 48–57.
119. Kalaiselvi, R., Muthukumarasamy, N., Velauthapillai, D., Kang, M., Senthila, T.S. *Mat. Lett.*, **2018**, *219* 198–200.
120. Kojima, A., Teshima, K., Shirai, Y., Miyasaka, T. *J. Am. Chem. Soc.,* **2009**, *131*, 6050–6051.
121. Zhou, H., Chen, Q., Li, G., Luo, S., Song, T.-B., Duan, H.-S., Hong, Z., You, J., Liu, Y.,Yang, Y. *Science,* **2014**, *345*, 542–546.
122. Stranks, S.D., Eperon, G.E., Grancini, G., Menelaou, C., Alcocer, M.J., Leijtens, T., Herz, L.M., Petrozza, A., Snaith, H.J. *Science,* **2013**, *342*, 341–344.
123. Mei, A., Li, X., Liu, L., Ku, Z., Liu, T., Rong, Y., Xu, M., Hu, M., Chen, J., Yang, Y. *Science,* **2014**, *345*, 295–298.
124. Wang, Y., Rho, W.-Y., Yang, H.-Y., Mahmoudi, T., Seo, S., Lee, D.-H., Hahn, Y.-B. *Nano Energy,* **2016**, *27*, 535–544.
125. Wang, Y., Mahmoudi, T., Rho, W.-Y., Yang, H.-Y., Seo, S., Bhat, K.S., Ahmad, R., Hahn, Y.-B. *Nano Energy,* **2017**, *40*, 408–417.
126. Yeo, J.-S., Kang, R., Lee, S., Jeon, Y.-J., Myoung, N., Lee, C.-L., Kim, D.-Y., Yun, J.-M.,Seo, Y.-H., Kim, S.-S. *Nano Energy,* **2015**, *12,* 96–104.
127. Jeng, J.Y., Chiang, Y.F., Lee, M.H., Peng, S.R., Guo, T.F., Chen, P., Wen, T.C. *Adv. Mater.,* **2013**, *25,* 3727–3732.
128. Liang, P.W., Liao, C.Y., Chueh, C.C., Zuo, F., Williams, S.T., Xin, X.K., Lin, J., Jen, A.K.Y. *Adv. Mater.,* **2014**, *26,* 3748–3754.
129. You, J., Hong, Z., Yang, Y.M., Chen, Q., Cai, M., Song, T.-B., Chen, C.-.C., Lu, S., Liu, Y., Zhou, H. **2014**.
130. Liu, X., Yu, H., Yan, L., Dong, Q., Wan, Q., Zhou, Y., Song, B., Li, Y. *ACS Appl. Mater. Interfaces,* **2015**, *7,* 6230–6237.
131. Qiu, W., Buffière, M., Brammertz, G., Paetzold, U.W., Froyen, L., Heremans, P., Cheyns, D. *Org. Electron.,* **2015**, *26,* 30–35.
132. Bai, Y., Yu, H., Zhu, Z., Jiang, K., Zhang, T., Zhao, N., Yang, S., Yan, H. *J. Mater. Chem., A* **2015**, *3*, 9098–9102.
133. Kuang, C., Tang, G., Jiu, T., Yang, H., Liu, H., Li, B., Luo, W., Li, X., Zhang, W., Lu, F. *Nano Lett.*, **2015**, *15,* 2756–2762.
134. Adam, G., Kaltenbrunner, M., Głowacki, E.D., Apaydin, D.H., White, M.S., Heilbrunner, H., Tombe, S., Stadler, P., Ernecker, B., Klampfl, C.W. *Sol. Energy Mater. Sol. Cells,* **2016**, *157*, 318–325.
135. Hou, F., Su, Z., Jin, F., Yan, X., Wang, L., Zhao, H., Zhu, J., Chu, B., Li, W. *Nanoscale,* **2015**, *7*, 9427–9432.
136. Huang, X., Wang, K., Yi, C., Meng, T., Gong, X. *Adv. Energy Mater.,* **2016**, *6*, 1501773.
137. Tavakoli, M.M., Tavakoli, R., Hasanzadeh, S., Mirfasih, M.H., *J. Phys. Chem. C.* **2016**, *120,* 19531–19536.

CHAPTER 5

FABRICATION TECHNIQUES OF SMART MATERIALS

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ABSTRACT

Smart materials have a tendency to change their physical and chemical characteristics in response to certain stimuli. These stimuli can be in terms of temperature, illumination, pressure, or magnetic and electric fields. This characteristic renders them highly versatile, finding utility in various domains including structural materials, actuators, sensors, and energy storage devices. These alloys can undergo deformation at one temperature and recover their original properties upon exposure to a distinct temperature. Similarly, piezoelectric ceramics demonstrate the conversion of mechanical stress into electric charge, making them valuable for generating ultrasonic waves, fabricating transducers, and enabling precise positioning actuators. Electrochromic materials respond to external bias by altering their color and are employed in display units and optoelectronic devices. Numerous synthesis techniques exist for fabricating smart materials, encompassing extrusion, injection molding, and more. Shape memory alloys can be prepared via diverse approaches such as powder metallurgy, rapid solidification, and casting. Smart materials possess the potential to revolutionize a wide array of industries, ranging from aerospace and automotive to biomedical and construction. Their distinctive properties and capability to undergo transformations in response to specific stimuli offer an extensive realm of possibilities for pioneering and innovative applications.

5.1 INTRODUCTION

Smart materials, also known as intelligent or responsive materials, are materials that possess unique properties that allow them to respond to changes in their environment in a predetermined and controlled manner. These materials can adapt to various stimuli, such as temperature, light, pressure, or moisture, to change their physical or chemical properties, and can even perform complex functions without external intervention [1]. The development of smart materials has revolutionized the fields of engineering, medicine, and materials science, providing new solutions to longstanding problems and opening up new possibilities for innovation and discovery [2]. Smart materials have found significant applications in the field of engineering, where they enable the creation of advanced structures and devices capable of adapting to dynamic conditions [3]. Notably, shape memory alloys (SMAs) exhibit the remarkable ability to alter their shape when subjected to variations in temperature or electrical current. This unique property renders them invaluable in a range of applications, including actuators, sensors, and artificial muscles. Their shape-shifting nature allows for precise control and responsiveness in various engineering systems.

Likewise, piezoelectric substances are those which generate electric charges with the application of applied stress. This characteristic empowers them to use piezoelectric materials in energy harvesting and sensor applications. These materials can efficiently harness mechanical forces and convert them into electrical signals, enabling the development of efficient energy systems and highly sensitive sensors [4]. In the realm of medicine, smart materials are making significant strides by contributing to be used in drug delivery systems and implantable devices that respond intelligently to changes within the body. For instance, smart hydrogels exhibit the remarkable ability to proclamate drugs with respect to fluctuations in pH level or temperature. This behavior enables the development of targeted drug delivery systems, where medications are released precisely at the desired location or under specific physiological conditions. Such systems hold immense promise for enhancing therapeutic outcomes and minimizing side effects. Furthermore, the integration of smart materials into implants, including bone scaffolds and stents, brings about transformative advancements in the field of medicine. These implants possess the capacity to adapt to changes in the body's environment, be it altering their shape or releasing drugs. By intelligently responding to physiological cues, they can enhance patient outcomes, reduce the need for invasive procedures, and provide more personalized and effective medical interventions. Smart materials are also finding applications in the field of consumer goods and electronics, where they are being used to develop new products with enhanced functionality and performance [5, 6].

Self-healing materials can repair themselves when damaged, making them useful in the development of more durable and long-lasting products [7]. Smart textiles can change color or shape in response to changes in the environment, making them useful in the development of responsive clothing and accessories [8].

Moreover, the development of smart materials has also opened up new possibilities for sustainability and environmental protection. For example, self-cleaning surfaces can reduce the need for harsh chemicals and cleaning agents, while smart coatings can reduce the need for frequent maintenance and repair. Smart materials are also being used to develop new energy-efficient systems and devices, helping to reduce carbon emissions and improve energy efficiency.

In this chapter, we will discuss a few of the existing smart materials and the different approaches opted for their synthesis.

5.2 TYPES OF SMART MATERIALS

Smart materials exhibit the special characteristics to modify their intrinsic features with the application of external stimuli. Diverse types of smart materials can be identified, including (Figure 5.1):

- Shape memory alloys (SMAs): These alloys demonstrate the capacity to undergo deformation upon a temperature change, followed by the capability to recover their initial shape.
- Piezoelectric materials: These substances induce generate an electric potential when subjected to mechanical stress and, conversely, experience dimensional alterations under the influence of an applied electric field.
- Thermochromic materials: Such materials manifest alterations in their coloration as a consequence of temperature variations.
- Electrochromic materials: These materials undergo color changes in response to an applied electric field.
- Magnetostrictive materials: Exhibiting sensitivity to magnetic fields, these materials experience modifications in their shape.
- Photochromic materials: These materials showcase color modifications upon exposure to light.
- pH-sensitive polymers: This category of materials undergoes alterations in shape or properties in response to changes in pH levels.

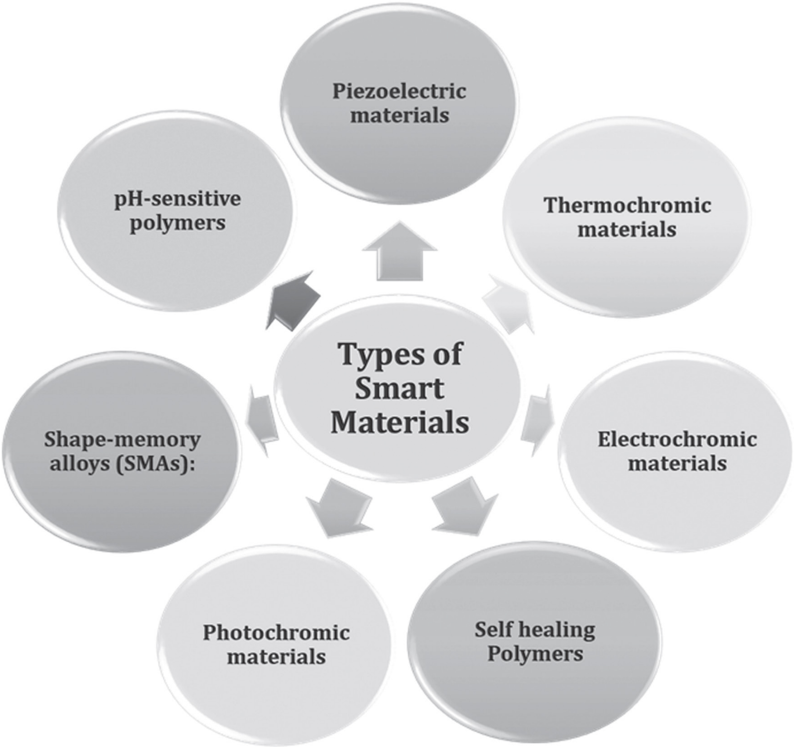
Piezoelectric materials
Thermochromic materials
Electrochromic materials
Self healing Polymers
Photochromic materials
Shape-memory alloys (SMAs):
pH-sensitive polymers
Types of Smart Materials

FIGURE 5.1 Types of smart materials. ⏎

5.3 SYNTHESIS ROUTES OF VARIOUS SMART MATERIALS

5.3.1 SHAPE-MEMORY POLYMERS (SMPS)

SMAs are a type of smart material that can “remember” their original shape and return to it when heated as shown in Figure 5.2. They are used in a variety of applications, including medical devices, aerospace, and consumer products.

Here are some common fabrication techniques for SMAs:

5.3.1.1 MELTING AND CASTING

This is a widely employed technique for the fabrication of SMAs. The process involves melting the alloy in a furnace and subsequently casting it into a mold. The resulting product undergoes heat treatment to achieve the desired shape memory effect. Notably, Ochin et al. conducted a study in which they synthesized multielementary alloys of A: B type, with A representing Ti, Hf, Zr, and B including Ni, Cu, Co, Pd, Ag, and Sn. These alloys were solidified into metallic glasses or partially crystalline amorphous phases, exhibiting superelastic characteristics typical of SMAs [9]. In a separate study, Silva et al. successfully designed NiTiAg SMAs using vacuum arc remelting. The developed melting procedure capitalized on the specific properties of Ni, Ti, and Ag to achieve alloy design and demonstrated the feasibility of producing chemically stable alloys [10].

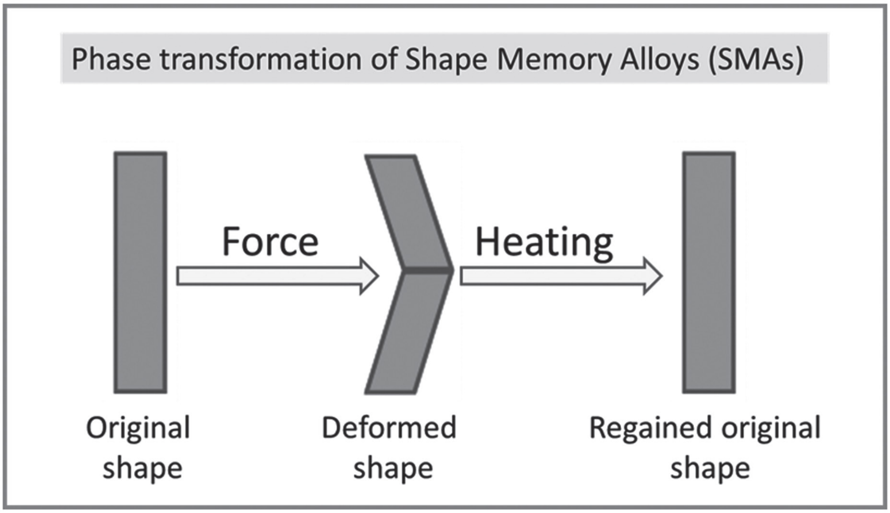

FIGURE 5.2 Illustration of shape memory alloy. ⏎

5.3.1.2 POWDER METALLURGY

In this technique, the SMA is first produced in the form of a fine powder. The powder is then compacted into a desired shape and sintered to form a solid piece. A. A. Atiyah et al. examined the impact of copper (Cu) additions of different weight percentages and compacting pressures (150–450 MPa) on the microstructure and physical characteristics of NiTi-based SMA produced by powder metallurgy [11]. Abdullah et al. presented a general overview of NiTi SMA processing using the traditional PM method, with the goal of helping to focus on porous parts that are appropriate for biomedical and implant applications [12].

5.3.1.3 COLD-WORKING

Cold-working is a process that involves deforming the SMA at room temperature by rolling, bending, or drawing. This process increases the strength and ductility of the material. Thermomechanical studies on NiTi SMA wire specimens that have been fully annealed and subsequently cold rolled to reduce the specimen width to 10%, 20%, and 40% of the initial wire diameter for 15 min were reported by Miller et al. [13]. For extensively cold-drawn Ti–Ni, the effects of cold-working and following low-temperature heat treatment on transformation temperatures and recovery strains were investigated by Otsuku et al. [14].

5.3.1.4 ADDITIVE MANUFACTURING

The techniques such as 3D printing, offer viable means to fabricate SMAs. This approach proves particularly advantageous for generating intricate shapes or components with internal structures. Among the additive manufacturing processes, laser powder bed fusion (L-PBF) stands out, demonstrating the capability to produce NiTi (Nitinol) SMAs with complex geometries and customizable functional properties. Zhu et al. conducted an investigation exploring the influence of hatch distance on the microstructure, phase transformation, and thermal cycling stability of NiTi alloys fabricated via the laser powder bed fusion process [15]. Additionally, the selective laser melting (SLM) additive manufacturing technique has been utilized to fabricate a NiTi-20Hf high-temperature SMA (HTSMA). Elahinia et al. conducted a comparative study examining the thermomechanical and shape memory response of this SLM-produced alloy in relation to its standard vacuum induction skull melting counterpart [16].

5.3.1.5 ELECTRODEPOSITION

Electrodeposition is a process involving the deposition of SMAs onto a substrate through electrochemical reactions. This technique holds considerable utility in the fabrication of thin films of SMAs, particularly for applications in microelectronics and biomedicine. Fricoteaux and Rousse conducted a study on the electrosynthesis of Cu–Zn, Al, and Cu–Zn–Al nanowires using the ionic liquid 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl) imide [17]. The composition of the Cu–Zn deposit exhibited an unexpected evolution in relation to polarization, attributed to the complex kinetics of the deposition process. In a separate investigation, Espiritu and Amorsolo successfully utilized an electrodeposition-annealing process to create Cu–Zn–Sn SMAs with average compositions of 56.0 at% Cu, 36.1 at% Zn, and 7.9 at% Sn. The resulting ternary alloys were subjected to flame tests to evaluate their shape memory response in terms of percent displacement (martensite phase recovery) [18].

5.3.2 PIEZOELECTRIC MATERIALS

Piezoelectric materials are smart materials that can generate an electrical charge in response to mechanical stress, or produce mechanical stress in response to an electrical charge as depicted in Figure 5.3. These materials are used in a variety of applications, including sensors, actuators, and energy harvesting. Here are some common fabrication techniques for piezoelectric materials:

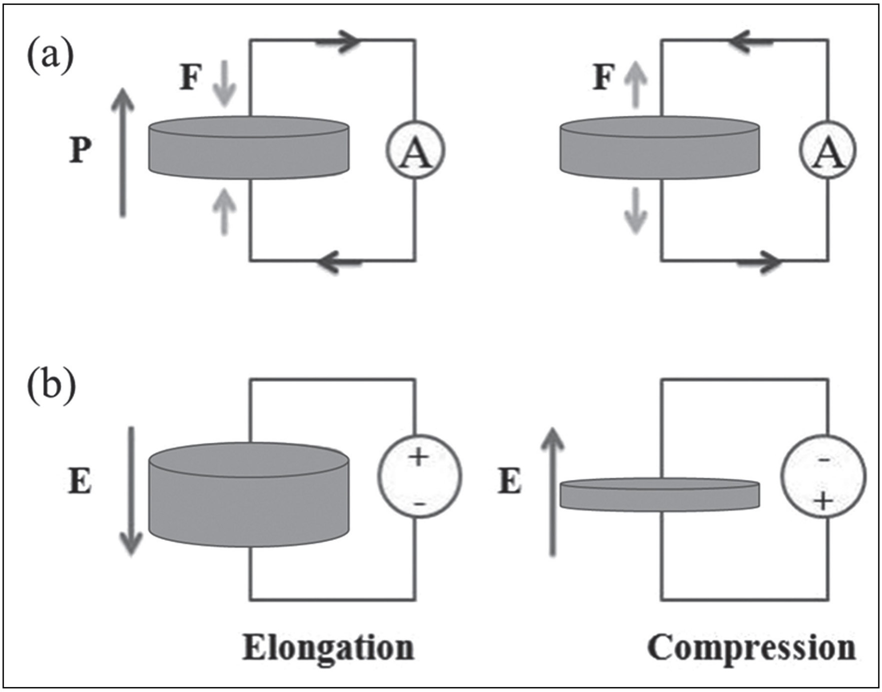

FIGURE 5.3 (a) Direct piezoelectric effect and (b) inverse piezoelectric effect. ⏎

5.3.2.1 SOLID-STATE REACTION

This method involves mixing the appropriate chemical precursors of the piezoelectric material and heating them at high temperatures. This results in a crystalline material with piezoelectric properties. From regular $BaCO_3$ and TiO_2 powders, high-piezoelectric coefficient $BaTiO_3$ ceramics have been produced successfully through the traditional solid-state reaction process by Shao et al. [19]. According to their investigation, the size of the domain wall is a crucial element that considerably affects the piezoelectric capabilities. The morphotropic phase boundary-near modified-PZT ceramics were made using a conventional method in a solid state. Kahoul et al. investigated their dielectric and piezoelectric properties for potential applications [20].

5.3.2.2 SOL–GEL PROCESSING

This method involves creating a solution of the precursor materials and depositing it onto a substrate. The solution is then heated to form a gel, which is then calcined at high temperatures to create a piezoelectric material. Praveen et al. studied piezoelectric properties of lead-free barium zirconium titanate-barium calcium titanate synthesized by sol–gel method. Solid-state sintering of the green pellets at 1550°C produced a highly dense and uniform microstructure with 95% of the predicted density [21]. In their further study, they investigated the impact of electric poling on the piezoelectric characteristics of sintered $[_x\text{BZT-}_{(1-x)}\text{BCT}]$ ceramics with different poling temperatures and poling fields. The outcomes showed that in order to improve the piezoelectric properties of $[_x\text{BZT-}_{(1-x)}\text{BCT}]$ ceramics, optimized poling conditions are needed [22].

5.3.2.3 CHEMICAL VAPOR DEPOSITION (CVD)

This technique involves the deposition of a thin film of piezoelectric material onto a substrate using chemical reactions in the gas phase. Ning et al. reported the opposite magnetoelectric effect in the heteroepitaxial structures of nickel ferrite $NiFe_2O_4$ (NFO) films grown on single crystals of lead zinc niobate-lead titanate (PZN-PT) or lead magnesium niobate-lead titanate (PMN-PT) substrates with a (001) orientation [23]. The ZnO micro-thornyballs (ZMTBs)-based piezoelectric nanogenerator was introduced by Yin et al. The CVD approach was used to create ZMTBs without the use of substrates or seed layers. The properties of the connections generated between the ZnO micro-thornyballs and the copper electrode were then revealed through electrical analysis [24].

5.3.2.4 ELECTROPHORETIC DEPOSITION

This method involves the deposition of a piezoelectric material from a suspension of charged particles under the influence of an electric field. By depositing two electrode-separated layers of PZT powder on the helix-shaped substrate and co-sintering, the electrophoretic deposition (EPD) technology was effectively used to create the helical actuator by Chen et al. [25]. Kim et al. used the traditional uniaxial pressing and EPD procedure to create lead-free $85(Bi_{0.5}Na_{0.5})TiO_3$-$15BaTiO_3$ (85BNT-15BT) piezoelectric ceramics. To produce thick green ceramics with an 85BNT-15BT composition using the EPD technique, many variables including suspension media, the applied electrical field, and deposition time were optimized [26].

5.3.2.5 LITHOGRAPHY

This technique involves patterning a substrate with a piezoelectric material using a lithographic mask and etching techniques. Marino et al. described the creation of structures suited for cell culture that were created using the two-photon polymerization of a nanocomposite resist. During synthesis, piezoelectric barium titanate nanoparticles have been added to the commercially available Ormocomp, and bio-inspired 3D structures resembling the trabeculae of sponge bone have been created [27].

5.3.2.6 HYDROTHERMAL SYNTHESIS

This method involves growing a piezoelectric material on a substrate using a high-pressure, high-temperature aqueous solution. Using a low-temperature hydrothermal method, Pb-free piezoelectric bismuth sodium titanate (BNT) nanostructures were created by Ghasemian et al. It is discovered that the precursors' composition and concentration, as well as the processing circumstances, have a significant impact on the products' phase and morphology. Well-crystallized BNT nanofibers with 150–200 nm diameters and less than 5 m in length were produced by adjusting the synthesis settings [28]. In their further studies, Ghasemian et al. reported hydrothermally created Pb-free

$Bi_{0.5}(Na_{0.8}K_{0.2})_{0.5}TiO_3$ nanotubes having a significant piezoelectric coefficient of 76 pm/V along the diameter direction, which is comparable to lead-based piezoelectrics. Without the use of a surfactant or template, the 30–50 nm diameter nanotubes are created through a scrolling and wrapping action [29].

5.3.3 THERMOCHROMIC MATERIALS

Thermochromic materials are those that change color in response to changes in temperature (Figure 5.4). These materials have a wide range of applications in fields such as sensors, smart windows, and textiles.

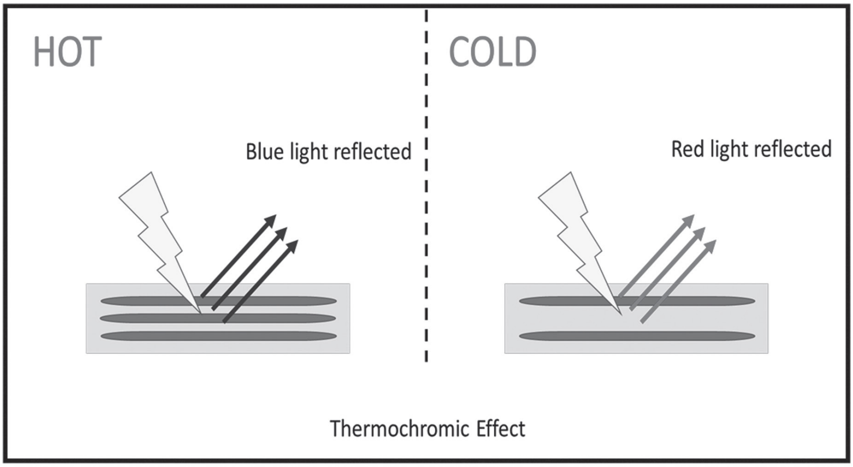

FIGURE 5.4 Schematic of thermochromic effect. ⏎

There are several different synthesis techniques for thermochromic materials, including:

5.3.3.1 SOL–GEL METHOD

This is a versatile and widely used method for preparing thermochromic materials. It involves the hydrolysis and condensation of metal alkoxides in a solvent to form a gel, which is then dried and calcined to produce the final product. Nguyen reported the synthesis of chromium-doped aluminum oxide via pechini sol–gel technique and explored its applications for reversible thermochromic sensors [30]. Carmona et al. reported that with varying solvent/

water ratios, anhydrous cobalt(II) chloride has been encapsulated in a number of inorganic sol–gel matrices. Sols were cast into hermetically sealed cuvettes. Sol–gel materials of this type were discovered to change color when exposed to temperatures between 10 and 50°C. By submerging the sensitive materials in a thermostatic water bath and recording the related visible spectra, the sensitive materials' general characteristics were determined. As the temperature rises, the optical reaction involves a shift in color from light pink to deep blue. The optical sensitivity of these temperature detectors in the aforementioned range is good, and they are reversible for more than 30 cycles [31].

5.3.3.2 CHEMICAL PRECIPITATION METHOD

This method involves the precipitation of metal ions from a solution by adding a precipitating agent. The resulting solid is then heated to produce the thermochromic material. Thermochromic vanadium dioxide (VO_2) thin film was deposited on a microscope glass substrate using the acidic chemical bath deposition (CBD) method using NH_4VO_3 as a vanadium source and the study was reported by Tsige et al. The potential of CBD-produced VO_2 thin films for applications in smart windows is demonstrated in the current investigations clearly in comparison to alternative synthesis methods [32].

5.3.3.3 CO-PRECIPITATION METHOD

This is a variation of the chemical precipitation method where two or more metal ions are precipitated simultaneously to form a mixed oxide material. This method can be used to tune the thermochromic properties of the material by controlling the composition. Silver cadmium tetraiodide Ag_2CdI_4 has two distinct functions: superionic and thermochromism. Ghanbari et al. synthesized Ag_2CdI_4/AgI nanocomposites using a straightforward in-situ co-precipitation technique. On the shape and purity of the products, the impact of several parameters including various capping agents and the molar ratio of Cd to Ag was examined [33].

5.3.3.4 SOLVOTHERMAL METHOD

This involves the reaction of metal salts in a high-pressure, high-temperature solvent to produce the thermochromic material. This method can produce materials with fine particle size and high purity. The synthesis and evaluation of extremely monodisperse, 7–10 nm-sized organically functionalized vanadium oxide (VOx) nanocrystals by solvothermal method have been reported by Jung et al. They exhibit good thermochromic characteristics after being thermally annealed at around 350°C, which is typical of VO_2 materials that go through a phase transition between low-temperature monocline VO_2(M) and high-temperature rutile VO_2(R) materials [34].

5.3.3.5 HYDROTHERMAL METHOD

This is similar to the solvothermal method but uses water as the solvent. This method is often used to prepare thermochromic materials with controlled morphology and crystal structure. In the study carried out by Wang, the rare earth RE/W-codoping has been proposed to improve the thermochromic performance of VO_2 by combining W's capacity to reduce transition temperature and RE's ability to increase T_{lum}/T_{sol} where T_{lum} is the integrated visible transmission and T_{sol} is the solar modulating ability. The hydrothermal assembly of the RE/W-codoped VO_2 nanoparticles was used to fabricate the thin film smart windows [35]. In another study, thermochromic properties of hydrothermally synthesized VO_2 were studied as a result of reversible structural transformation between tetragonal and monoclinic phases of VO_2 by Alie et al. [36].

5.3.3.6 ELECTROCHEMICAL DEPOSITION

This method involves the deposition of metal ions onto a substrate using an electric current. The deposited material can then be heat treated to produce the thermochromic material. Cheng et al. presented a review on thermochromic materials' classification, discoloration mechanism, and preparation techniques including electrochemical deposition, application domains, and development trends [37].

5.3.3.7 SPRAY PYROLYSIS METHOD

This method involves the decomposition of metal-containing precursors in a heated spray to produce the thermochromic material. This method can produce materials with a wide range of compositions and particle sizes. Aerosol spray pyrolysis was used to create nanostructured films of vanadium oxide (V_xO_y)

using varying precursor solution concentrations (0.005M, 0.01M, and 0.02M). Ammonium metavanadate (NH_4VO_3) was used as the precursor. The glass substrates (Corning glass) were subjected to the deposition at two distinct substrate temperatures (300°C and 400°C) [38].

5.3.4 ELECTROCHROMIC MATERIALS

Electrochromic materials are materials that can change color in response to an electric current or voltage as shown in Figure 5.5. The fabrication techniques of electrochromic materials vary depending on the specific material being used.

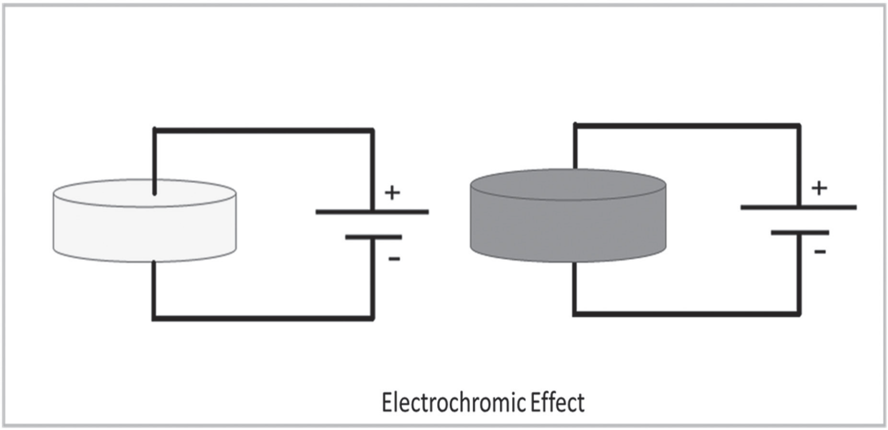

FIGURE 5.5 Illustration of electrochromic effect. ⏎

Here are some common techniques used to fabricate electrochromic materials as discussed below:

5.3.4.1 SOL–GEL METHOD

This technique involves the formation of a gel-like material by the hydrolysis of metal alkoxides. The gel is then processed to form a thin film on a substrate. This method is often used to fabricate electrochromic metal oxides, such as tungsten oxide and titanium oxide. In a recent study carrired out by Liu et al., tetrabutyl titanate was used as the starting material, niobium chloride as the dopant, methanol as the solvent and acetylacetone as the chelating agent to create Nb-doped TiO_2 films on ITO glass substrates by dip coating.

Studies have been done on how Nb doping affects the microstructure and electrochromic characteristics [39]. In order to create the complimentary electrochromic smart windows, sol–gel-coated WO_3 sheets were used in another study by Puroshothamam et al. [40].

5.3.4.2 CHEMICAL VAPOR DEPOSITION (CVD)

CVD is a technique that involves the deposition of a thin film on a substrate by the chemical reaction of gases. This technique is often used to fabricate electrochromic materials based on organic polymers, such as polyaniline. Kondrateva et al. reported the role played by structure on electrochromic behavior of nickel oxide thin coatings deposited on ITO-coated glass using CVD technique [41].

5.3.4.3 SPIN COATING

This technique involves the deposition of a thin film on a substrate by spinning a solution of the electrochromic material onto the substrate. This method is often used to fabricate electrochromic materials based on organic compounds, such as viologens. NiO thin films with solution processing have been created using the spin coating method. For the purpose of depositing layers of NiO solution on the FTO substrate, nickel nitrate hexahydrate and 2-aminoethanol have been utilized as the precursor and oxidizing agent for nickel, respectively, investigating how NiO layers affect morphological, structural, and electrochromic characteristics [42]. Sol–gel and spin coating were used to deposit nickel oxide thin films. This study described how NiO thin films' structural, morphological, and electrochromic properties are affected by the precursor's concentration, type of solvent, stabilizer, and final treatment (calcination or UV treatment) [43].

5.3.4.4 SPUTTERING

Sputtering is a technique that involves the deposition of a thin film on a substrate by bombarding the electrochromic material with high-energy particles. This method is often used to fabricate electrochromic metal films, such as tungsten oxide. One-step magnetron sputtering process was used to fabricate Sn-NiO films for a superior electrochromic performance. The amount of Sn in the Sn-NiO films was regulated by altering the sputtering power of the target SnO_2. The microstructure of the NiO film was modified due to Sn^{4+} ions which resulted in refinement of the grain size, promoting the diffusion of lithium ions and enlarging electrochemically active surface and hence improving the NiO film electrochromic performances [44].

5.3.4.5 INKJET PRINTING

Inkjet printing is a technique that involves the deposition of a thin film on a substrate by printing the electrochromic material using an inkjet printer. This method is often used to fabricate electrochromic materials based on organic compounds, such as polyaniline. In a recent study, Huang et al. presented flexible, patterned, and inkjet-printed electrochromic devices made of two-dimensional (2D) polyaniline (PANI) sheets that are uniformly disseminated in formic acid (FA), allowing for high precision, stable inkjet printing. The printed PANI electrodes and ECDs exhibit outstanding performance due to the immaculate lamellar structure of PANI sheets, which combines nanoscale thickness and an optimum doping ratio [45].

5.3.5 SELF-HEALING POLYMERS

Self-healing materials are materials that can repair themselves after damage without the need for external intervention (Figure 5.6). The fabrication techniques for self-healing materials depend on the specific material being used.

The following techniques can be used to synthesize self-healing materials:

5.3.5.1 MICROENCAPSULATION

Microencapsulation is a technique that involves the encapsulation of a healing agent in tiny capsules that are dispersed throughout the material. When the material is damaged, the capsules rupture, releasing the healing agent, which then fills the crack or defect in the material. The healing agent's microencapsulation technique has made it possible for the polymer material to do self-healing. Using a solvent evaporation approach, a new microcapsule containing tris(dimethylaminomethyl)phenol (DMP-30) with polystyrene as the shell material was created [46].

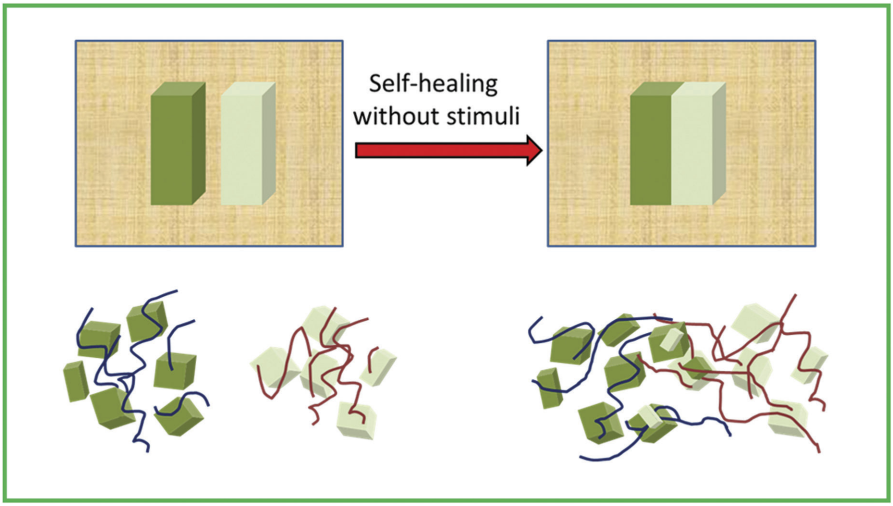

FIGURE 5.6 Pictorial view of self-healing materials. ⏎

5.3.5.2 SELF-ASSEMBLY

Self-assembly is a technique that involves the use of molecular interactions to create structures that can repair themselves. For example, materials can be designed with molecular components that can spontaneously form reversible bonds, allowing the material to heal itself after damage. Wang et al suggested a microscale/nanoscale assembly method based on noncovalent bonding-driven self-assembly of 2D nanosheets into an interwoven network to create extremely robust self-healing materials. The resultant composites have noticeably increased mechanical characteristics and self-healing efficiency, as well as outstanding functional-healing ability of the produced flexible devices, thanks to the interwoven network coupled by dense hydrogen bonds aggregated at the interface [47].

5.3.5.3 SHAPE-MEMORY POLYMERS

Shape-memory polymers are polymers that can change shape in response to an external stimulus, such as heat. When the polymer is damaged, the shape-memory effect can be used to repair the material by heating it to its original shape. Chen et al. presented a study wherein, the PCL/TPU blends are simply blended to create a form memory matrix. The poly(ε-caprolactone) and thermoplastic polyurethane (PCL/TPU) blends were then added with polydopamine (PDA) nanospheres acting as photothermal fillers, allowing the system to demonstrate exceptional light-response shape memory effect with a form recovery ratio of 100%. Additionally, the nanocomposites' microporous nature gives them good self-healing abilities [48].

5.3.5.4 POLYMERIZATION

Polymerization is a technique that involves the formation of a polymer from monomers. Self-healing polymers can be designed with monomers that can form reversible bonds, allowing the material to repair itself after damage. Li et al. developed and created a polymer/graphene-based self-healing material with a cross-linking network topology using the Diels–Alder (D–A) reaction. Under the influence of heat, infrared light, and microwaves while regulating the formation and cleavage of D–A bonds, the as-prepared material can be repaired after damage. Additionally, it demonstrates efficient (efficiencies are 90% after heat-healing, 106% after IR-healing, and 133% after microwave-healing, respectively), quick (IR light-5 s, Heat/Microwave-60s), and multichannel self-healing capabilities (i.e., may be self-healed in many ways) [49].

5.3.5.5 THREE-DIMENSIONAL (3D) PRINTING

3D printing is a technique that involves the layer-by-layer deposition of materials to create complex structures. Self-healing materials can be designed with embedded healing agents, allowing the material to repair itself after damage. With a focus on reforming reactions and carbon adsorption and how effective it could be in improving their performance, Soliman et al. presented an outline of how additive manufacturing is connected to the chemistry of catalysis and separation [50].

5.3.6 PHOTOCHROMIC MATERIALS

Photochromic materials are materials that change their color or optical properties in response to light, particularly in the UV or visible spectrum (Figure 5.7). The fabrication methods of photochromic materials depend on the specific material being used.

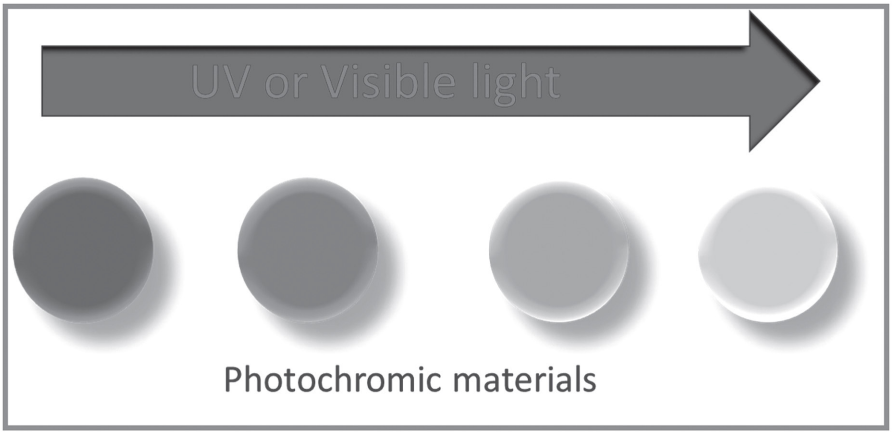

FIGURE 5.7 Representation of photochromic materials. ⏎

There exist numerous methods to fabricate photochromic materials, a few of them are discussed below:

5.3.6.1 SOL–GEL METHOD

This technique involves the formation of a gel-like material by the hydrolysis of metal alkoxides. The gel is then processed to form a thin film on a substrate. This method is often used to fabricate photochromic metal oxides, such as titanium dioxide. In a recent report, sol–gel process has been used to produce a transparent glass that is photoluminescent by simply immobilizing alkaline earth aluminate nanoparticles. Under UV light, the glass substrates were demonstrated to become green [51]. In another study, thick films of potassium sodium niobate doped with Er^{3+} that exhibit room-temperature self-recovery photochromism were created, thereby broadening the range of materials that could exhibit this property and facilitating both theoretical research and practical application [52].

5.3.6.2 CHEMICAL VAPOR DEPOSITION (CVD)

CVD is a technique that involves the deposition of a thin film on a substrate by the chemical reaction of gases. This technique is often used to fabricate photochromic materials based on organic polymers, such as spiropyran derivatives. Burk et al. described the successful copolymerization and in-depth analysis of films made of hydroxyethyl methacrylate (HEMA) and cross-linked with a photoswitchable diazocine using initiated chemical vapor deposition (iCVD). Authors demonstrated the application of our films to several substrates, including glass and flexible polymeric materials, and he presented a simple method for patterning coatings using a shadow mask. It was possible to produce precise patterns in real time using a regular blue laser to induce photoswitching, demonstrating the usefulness of our films in industries like smart surfaces, labeling, or data storage [53].

5.3.6.3 SPIN COATING

This technique involves the deposition of a thin film on a substrate by spinning a solution of the photochromic material onto the substrate. This method is often used to fabricate photochromic materials based on organic compounds, such as azobenzene derivatives. Ulrich et al. used a modular thiol-ene resin as an interface along with nanoscale 3D printing for the fabrication of visible light-responsive photochromic 3D microobjects [54].

5.3.6.4 ELECTROCHROMIC DEPOSITION

Electrochromic deposition is a technique that involves the deposition of the photochromic material onto a substrate using an electrochemical process. A current is applied to the substrate to promote the deposition of the photochromic material onto the substrate. Shchegolkov et al. in their study generated WO_3 films by various techniques, including electrochemical deposition, magnetron sputtering, and explored electrochromic technologies. In their work, an illustration of an electrochromic “Smart Window” based on WO_3 has been provided. Various applications for electrochromic devices based on nanostructured materials are examined in contemporary analysis [55].

5.3.7 pH-SENSITIVE POLYMERS

pH-sensitive polymers are polymers that change their physical or chemical properties in response to changes in pH. The fabrication techniques for pH-sensitive polymers depend on the specific polymer being used.

The following methods can be utilized to prepare pH-sensitive materials:

5.3.7.1 EMULSION POLYMERIZATION

Emulsion polymerization is a technique that involves the polymerization of monomers in an aqueous emulsion. pH-sensitive monomers can be incorporated into the emulsion and polymerized to form pH-sensitive polymers. The resulting polymer particles can be used as colloidal carriers for drug delivery or as pH-responsive materials in sensing applications. Abandansari et al. reported the creation of a novel pH-sensitive H40-based nanogel structure using a click reaction and mini-emulsion polymerization. These nanogels are pH-sensitive, and their swelling ratio closely relates to the environment's pH. This intracellular delivery technique involved exposing the nanogel to low-pH cytosol conditions, which caused the nanogel to swell and release the medication [56].

5.3.7.2 SOLUTION POLYMERIZATION

Solution polymerization is a technique that involves the polymerization of monomers in a solvent. pH-sensitive monomers can be incorporated into the solvent and polymerized to form pH-sensitive polymers. The resulting polymer can be used in a variety of applications, such as coatings, adhesives, and membranes. A study based on a novel pH-sensitive sulfonamide, sulfadimethoxine (SD; 6.1 pK_a), or a polymer (PSD; Mw: 3000) of its derivative used to modify the end of polymeric micelles made of block copolymers of poly(L-lactide) (PLLA) and poly(ethylene glycol) (PEG) has been reported by Han et al. [57]. By employing 2-aminoethanethiol as a chain transfer agent, a vinylated SD (SD monomer; SDM) was radically polymerized to create PSD.

5.3.7.3 ELECTROSPINNING

Electrospinning is a technique that involves the application of a high voltage to a polymer solution, resulting in the formation of a polymer fiber. pH-sensitive monomers can be incorporated into the polymer solution, and the resulting fibers can be used in a variety of applications, such as tissue engineering and drug delivery. A novel pH-sensitive polymer/lipid nanocomposite was created using a modified tri-axial electrospinning technique by Yang et al. A model of weakly water-soluble medication can be encouraged to dissolve and permeate using the systems created [58].

5.3.7.4 LAYER-BY-LAYER ASSEMBLY

Layer-by-layer assembly is a technique that involves the deposition of alternating layers of positively and negatively charged polymers onto a substrate. pH-sensitive polymers can be incorporated into the assembly, and the resulting multilayered films can be used in a variety of applications, such as sensing and drug delivery. Ulasevich et al. presented a straightforward idea of a light-induced pH change and then manipulated the mechanical characteristics of a nearby polymer sheet at high amplitudes. It is known that radiation of a titania surface causes water to split, and that this can be exploited to bring the pH of the surrounding environment down to 4. Thus, a nearby pH-sensitive polymer film's mechanical modulus can change by more than an order of magnitude [59].

5.3.7.5 CHEMICAL MODIFICATION

Chemical modification is a technique that involves the modification of a polymer's chemical structure to make it pH-sensitive. This can be achieved by incorporating pH-sensitive groups into the polymer backbone or by modifying existing functional groups to make them pH-sensitive. Banks et al. reported two techniques for chemically modifying alginate to produce a hydrogel with neutral-basic pH sensitivity. In the first technique, 4-(2-aminoethyl) benzoic acid and alginate directly form an amide bond. Reductive amination of oxidized alginate is the second technique that was developed in an effort to better control the alginate hydrogel's rate of deterioration. Both techniques produce a hydrogel vehicle for targeted delivery of encapsulated payload in the gastrointestinal tract under physiological conditions [60].

5.4 CONCLUSION

In conclusion, the development of smart materials has revolutionized the field of materials science and engineering. SMAs, electrochromic materials, and piezoelectric materials are examples of smart materials that have shown tremendous potential in various applications, from biomedical implants to energy-efficient windows. The different fabrication techniques available for these materials offer a range of options for researchers and engineers to tailor their properties and characteristics to suit specific application requirements. While each technique has its advantages and limitations, the continuous advancements in fabrication technologies are enabling the production of smarter and more versatile materials. As research continues in this field, we can expect to see even more innovative applications of smart materials in the future.

Moreover, the integration of smart materials with other technologies such as sensors, actuators, and control systems is opening up new possibilities for the development of intelligent structures and systems. The ability of these materials to sense, respond, and adapt to changes in their environment makes them attractive for use in a wide range of fields, including aerospace, robotics, and civil engineering. As we continue to explore the potential of smart materials and their fabrication techniques, it is clear that they will play an increasingly important role in shaping the future of materials science and engineering. However, the development and use of smart materials also raise important ethical and social questions that must be addressed. For example, the use of smart materials in military applications raises concerns about the development of autonomous weapons, while the use of smart materials in consumer goods and electronics raises concerns about privacy and data security.

KEYWORDS

- **smart materials**
- **stimuli-responsive materials**
- **adaptive materials**
- **shape memory alloys**
- **piezoelectric materials**
- **electrochromic materials**
- **thermochromic materials**

REFERENCES

1. Yin, Y., Rogers, J.A. Introduction: smart materials. *Chem. Rev.*, **2022**, *122*(5), 4885–4886.
2. Drossel, W.G., Kunze, H., Bucht, A., Weisheit, L., Pagel, K. Smart3–Smart materials for smart applications. *Procedia Cirp.*, **2015**, *36*, 211–216.
3. Rana, S., Subramani, P., Fangueiro, R., Correia, A.G. A review on smart self-sensing composite materials for civil engineering applications. *AIMS Mater. Sci.*, **2016**, *3*(2), 357–379.

4. Shukla, U., Garg, K. Journey of smart material from composite to shape memory alloy (SMA), characterization and their applications—a review. *Smart. Mater. Med.*, **2023**, *4*, 227–242.
5. Asapur, P.C., Banerjee, I. Smart materials for medical applications. In *Polymer nanocomposite-based smart materials*, Woodhead Publishing, 2020, pp. 177–196.
6. Popa, L., Ghica, M.V., Dinu-Pirvu, C. (Eds.). *Hydrogels: smart materials for biomedical applications*, BoD–Books on Demand, 2019.
7. Chen, J., Huang, Y., Ma, X., Lei, Y. Functional self-healing materials and their potential applications in biomedical engineering. *Adv. Compos. Mater.*, **2018**, *1*, 94–113.
8. Çelikel, D.C. Smart e-textile materials. In *Advanced functional materials*, **2020**, pp. 1–16.
9. Ochin, P., Kolomytsev, V., Pasko, A., Sezonenko, A., Vermaut, P., Prima, F., Portier, R. Amorphous multielementary alloys: a preparation route for shape memory alloys. *J. Alloys Compd.*, **2007**, *434*, 268–271.
10. Álvares da Silva, G.H., Otubo, J. Designing NiTiAg shape memory alloys by vacuum arc remelting: first practical insights on melting and casting. *Shape. Mem. Superelasticity*, **2018**, *4*, 402–410.
11. Atiyah, A.A., Ali, A.R.K.A., Dawood, N.M. Characterization of NiTi and NiTiCu porous shape memory alloys prepared by powder metallurgy (Part I). *Arab. J. Sci. Eng.*, **2015**, *40*, 901–913.
12. Abdullah, Z., Razali, R., Subuki, I., Omar, M.A., Ismail, M.H. An overview of Powder Metallurgy (PM) method for porous nickel-titanium shape memory alloy (SMA). *Adv. Mater. Res.*, **2016**, *1133*, 269–274.
13. Miller, D.A., Lagoudas, D.C. Influence of cold work and heat treatment on the shape memory effect and plastic strain development of NiTi. *Mater. Sci. Eng. A.*, **2001**, *308*(1–2), 161–175.
14. Xu, Y., Otsuka, K., Toyama, N., Yoshida, H., Nagai, H., Kishi, T. Additive nature of recovery strains in heavily cold-worked shape memory alloys. *Scr. Mater.*, **2003**, *48*(6), 803–808.
15. Zhu, J.N., Borisov, E., Liang, X., Huizenga, R., Popovich, A., Bliznuk, V., ... Popovich, V. Controlling microstructure evolution and phase transformation behavior in additive manufacturing of nitinol shape memory alloys by tuning hatch distance. *J. Mater. Sci.*, **2022**, *57*(10), 6066–6084.
16. Elahinia, M., Moghaddam, N.S., Amerinatanzi, A., Saedi, S., Toker, G.P., Karaca, H., ... Benafan, O. Additive manufacturing of NiTiHf high temperature shape memory alloy. *Scr. Mater.*, **2018**, *145*, 90–94.
17. Fricoteaux, P., Rousse, C. Nanowires of Cu–Zn and Cu–Zn–Al shape memory alloys elaborated via electrodeposition in ionic liquid. *J. Electroanal. Chem.*, **2014**, *733*, 53–59.
18. Espiritu, R., Amorsolo, A. Fabrication and characterization of Cu–Zn–Sn shape memory alloys via an electrodeposition–annealing route. *Int. J. Miner. Metall. Mater.*, **2019**, *26*, 1436–1449.
19. Shao, S., Zhang, J., Zhang, Z., Zheng, P., Zhao, M., Li, J., Wang, C. High piezoelectric properties and domain configuration in $BaTiO_3$ ceramics obtained through the solid-state reaction route. *J. Phys. D: Appl. Phys.*, **2008**, *41*(12), 125408.
20. Kahoul, F., Hamzioui, L., Guemache, A., Aillerie, M., Boutarfaia, A. Study of dielectric and piezoelectric properties of (1−x) PZT-xSFN ceramics prepared by conventional solid state reaction method. *J. Chem. Soc. Pak.*, **2020**, *42*(5), 634–638.
21. Praveen, J.P., Kumar, K., James, A.R., Karthik, T., Asthana, S., Das, D. Large piezoelectric strain observed in sol–gel derived BZT–BCT ceramics. *Curr. Appl. Phys.*, **2014**, *14*(3), 396–402.

22. Praveen, J.P., Karthik, T., James, A.R., Chandrakala, E., Asthana, S., Das, D. Effect of poling process on piezoelectric properties of sol–gel derived BZT–BCT ceramics. *J. Eur. Ceram. Soc.*, **2015**, *35*(6), 1785–1798.
23. Li, N., Liu, M., Zhou, Z., Sun, N.X., Murthy, D.V.B., Srinivasan, G., ... Gupta, A. Electrostatic tuning of ferromagnetic resonance and magnetoelectric interactions in ferrite-piezoelectric heterostructures grown by chemical vapor deposition. *Appl. Phys. Lett.*, **2011**, *99*(19), 192502.
24. Yin, B., Qiu, Y., Zhang, H., Ji, J., Lei, J., Luo, Y., ... Hu, L. Piezoelectric nanogenerator with 3D-ZnO micro-thornyballs prepared by chemical vapour deposition. *J. Mater. Sci. Mater. Electron.*, **2015**, *26*, 742–746.
25. Chen, Y.H., Li, T., Boey, F.Y.C., Ma, J. Electrophoretic deposition and characterization of helical piezoelectric actuator. *Ceram. Int.*, **2008**, *34*(1), 1–6.
26. Kim, M., Ito, R., Kim, S., Khanal, G.P., Fujii, I., Suzuki, T.S., Uchikoshi, T., Moriyoshi, C., Kuroiwa, Y., Wada, S. Fabrication of lead-free piezoelectric (Bi0. 5Na0. 5) TiO_3–$BaTiO_3$ ceramics using electrophoretic deposition. *J. Mater. Sci.*, **2018**, *53*(4), 2396–2404.
27. Marino, A., Barsotti, J., de Vito, G., Filippeschi, C., Mazzolai, B., Piazza, V., ... Ciofani, G. Two-photon lithography of 3D nanocomposite piezoelectric scaffolds for cell stimulation. *ACS Appl. Mater. Interfaces.*, **2015**, *7*(46), 25574–25579.
28. Ghasemian, M.B., Lin, Q., Adabifiroozjaei, E., Wang, F., Chu, D., Wang, D. Morphology control and large piezoresponse of hydrothermally synthesized lead-free piezoelectric (Bi 0.5 Na 0.5) TiO_3 nanofibres. *RSC Adv.*, **2017**, *7*(25), 15020–15026.
29. Ghasemian, M.B., Rawal, A., Liu, Y., Wang, D. Approaching piezoelectric response of Pb-piezoelectrics in hydrothermally synthesized Bi0. 5 (Na1–x K x) 0.5 TiO_3 nanotubes. *ACS Appl. Mater. Interfaces.*, **2018**, *10*(24), 20816–20825.
30. Nguyen, D.K., Bach, Q.V., Kim, B., Lee, H., Kang, C., Kim, I.T. Synthesis of Cr-doped Al2O3 by Pechini sol-gel method and its application for reversible thermochromic sensors. *Mater. Chem. Phys.*, **2019**, *223*, 708–714.
31. Carmona, N., Herrero-Hernandez, E., Llopis, J., Villegas, M.A. Novel sol–gel reversible thermochromic materials for environmental sensors. *J. Sol-Gel Sci. Technol.*, **2008**, *47*, 31–37.
32. Tsige, A., Ganesh, T., Mensur, D., Tesfaye, D. Thermal studies on chemical bath deposited thermochromic VO_2 thin film for energy efficient glass windows. *Mater. Today: Proc.*, **2021**, *45*, 6171–6175.
33. Ghanbari, M., Soofivand, F., Salavati-Niasari, M. Simple synthesis and characterization of Ag2CdI4/AgI nanocomposite as an effective photocatalyst by co-precipitation method. *J. Mol. Liq.*, **2016**, *223*, 21–28.
34. Jung, Y.H., Pack, S.P., Chung, S. Solvothermal synthesis and characterization of highly monodisperse organically functionalized vanadium oxide nanocrystals for thermochromic applications. *Mater. Res. Bull.*, **2018**, *101*, 67–72.
35. Wang, N., Goh, Q.S., Lee, P.L., Magdassi, S., Long, Y. One-step hydrothermal synthesis of rare earth/W-codoped VO_2 nanoparticles: reduced phase transition temperature and improved thermochromic properties. *J. Alloys Compd.*, **2017**, *711*, 222–228.
36. Alie, D., Gedvilas, L., Wang, Z., Tenent, R., Engtrakul, C., Yan, Y., ... Ban, C. Direct synthesis of thermochromic VO_2 through hydrothermal reaction. *J. Solid. State. Chem.*, **2014**, *212*, 237–241.
37. Cheng, Y., Zhang, X., Fang, C., Chen, J., Wang, Z. Discoloration mechanism, structures and recent applications of thermochromic materials via different methods: a review. *J. Mater. Sci. Technol.*, **2018**, *34*(12), 2225–2234.

38. Gavalas, S., Gagaoudakis, E., Katerinopoulou, D., Petromichelaki, V., Wight, S., Wotring, G., Aperathitis, E., Kiriakidis, G., Binas, V. Vanadium oxide nanostructured thin films prepared by aerosol spray pyrolysis for gas sensing and thermochromic applications. *Mater. Sci. Semicond.*, **2019**, *89*, 116–120.
39. Liu, R., Ren, Y., Wang, J., Wang, Y., Jia, J., Zhao, G. Preparation of Nb-doped TiO2 films by sol-gel method and their dual-band electrochromic properties. *Ceram. Int.*, **2021**, *47*(22), 31834–31842.
40. Purushothaman, K.K., Muralidharan, G., Vijayakumar, S. Sol-gel coated WO_3 thin films based complementary electrochromic smart windows. *Mater. Lett.*, **2021**, *296*, 129881.
41. Kondrateva, A., Bespalova, P., Baryshev, G.K., Mishin, M. Electrochromic properties of NiO thin coatings. In *Key engineering materials*, Trans Tech Publications Ltd, 2019, Vol. 822, pp. 781–786.
42. Goel, R., Jha, R., Ravikant, C. Solution-processed spin coated multilayer structured nickel oxide thin films for anodic electrochromism. *J. Appl. Electrochem.*, **2023**, *53*(4), 713–735.
43. Zrikem, K., Song, G., Aghzzaf, A.A., Amjoud, M., Mezzane, D., Rougier, A. UV treatment for enhanced electrochromic properties of spin coated NiO thin films. *Superlattices Microstruct.*, **2019**, *127*, 35–42.
44. Zhao, Y., Zhang, X., Chen, X., Li, W., Wang, L., Li, Z., ... Li, Y. Preparation of Sn-NiO films and all-solid-state devices with enhanced electrochromic properties by magnetron sputtering method. *Electrochim. Acta.*, **2021**, *367*, 137457.
45. Huang, X., Chen, J., Xie, H., Zhao, F., Fan, S., Zhang, Y. Inkjet printing of 2D polyaniline for fabricating flexible and patterned electrochromic devices. *Sci. China. Mater.*, **2022**, *65*(8), 2217–2226.
46. Santos, A.N., Santos, D.J.D., Carastan, D.J. Microencapsulation of reactive isocyanates for application in self-healing materials: a review. *J. Microencapsul.*, **2021**, *38*(5), 338–356.
47. Wang, Y., Huang, X., Zhang, X. Ultrarobust, tough and highly stretchable self-healing materials based on cartilage-inspired noncovalent assembly nanostructure. *Nat. Commun.*, **2021**, *12*(1), 1291.
48. Chen, Y., Zhao, X., Luo, C., Shao, Y., Yang, M.B., Yin, B. A facile fabrication of shape memory polymer nanocomposites with fast light-response and self-healing performance. *Compos. A: Appl. Sci. Manuf.*, **2020**, *135*, 105931.
49. Li, G., Xiao, P., Hou, S., Huang, Y. Rapid and efficient polymer/graphene-based multichannel self-healing material via Diels-Alder reaction. *Carbon*, **2019**, *147*, 398–407.
50. Soliman, A., AlAmoodi, N., Karanikolos, G.N., Doumanidis, C.C., Polychronopoulou, K. A review on new 3-D printed materials' geometries for catalysis and adsorption: paradigms from reforming reactions and CO_2 capture. *Nanomaterials*, **2020**, *10*(11), 2198.
51. Al-Qahtani, S.D., Alzahrani, S.O., Snari, R.M., Al-Ahmed, Z.A., Alkhamis, K., Alhasani, M., El-Metwaly, N.M. Preparation of photoluminescent and photochromic smart glass window using sol-gel technique and lanthanides-activated aluminate phosphor. *Ceram. Int.*, **2022**, *48*(12), 17489–17498.
52. Lu, Y., Lin, J., Wang, P., Yu, F., Wu, X., Lin, C., ... Zhang, Q. Self-recoverable photochromism of tape-casting-derived Er-doped potassium sodium niobate thick films via sol-gel route. *J. Lumin.*, **2022**, *247*, 118875.
53. Burk, M.H., Langbehn, D., Hernández Rodríguez, G., Reichstein, W., Drewes, J., Schröder, S., Rehders, S., Strunskus, T., Herges, R., Faupel, F. Synthesis and investigation of a photoswitchable copolymer deposited via initiated chemical vapor deposition for application in organic smart surfaces. *ACS Appl. Polym. Mater.*, **2021**, *3*(3), 1445–1456.

54. Ulrich, S., Wang, X., Rottmar, M., Rossi, R.M., Nelson, B.J., Bruns, N., ... Boesel, L.F. Nano-3D-printed photochromic micro-objects. *Small*, **2021**, *17*(26), 2101337.
55. Shchegolkov, A.V., Jang, S.H., Shchegolkov, A.V., Rodionov, Y.V., Sukhova, A.O., Lipkin, M.S. A brief overview of electrochromic materials and related devices: a nanostructured materials perspective. *Nanomaterials*, **2021**, *11*(9), 2376.
56. Abandansari, H.S., Nabid, M.R., Rezaei, S.J.T., Niknejad, H. pH-sensitive nanogels based on Boltorn® H40 and poly(vinylpyridine) using mini-emulsion polymerization for delivery of hydrophobic anticancer drugs. *Polymer*, **2014**, *55*(16), 3579–3590.
57. Han, S.K., Na, K., Bae, Y.H. Sulfonamide based pH-sensitive polymeric micelles: physicochemical characteristics and pH-dependent aggregation. *Coll. Surf. A. Physicochem. Eng. Asp.*, **2003**, *214*(1–3), 49–59.
58. Yang, C., Yu, D.G., Pan, D., Liu, X.K., Wang, X., Bligh, S.A., Williams, G.R. Electrospun pH-sensitive core–shell polymer nanocomposites fabricated using a tri-axial process. *Acta. Biomater.*, **2016**, *35*, 77–86.
59. Ulasevich, S.A., Brezesinski, G., Möhwald, H., Fratzl, P., Schacher, F.H., Poznyak, S.K., Andreeva, D.V., Skorb, E.V. Light-induced water splitting causes high-amplitude oscillation of pH-sensitive layer-by-layer assemblies on TiO_2. *Angew. Chem.*, **2016**, *128*(42), 13195–13198.
60. Banks, S.R., Enck, K., Wright, M., Opara, E.C., Welker, M.E. Chemical modification of alginate for controlled oral drug delivery. *J. Agric. Food Chem.*, **2019**, *67*(37), 10481–10488.

PART II
Classification of Smart Materials

CHAPTER 6

MACHINE LEARNING FOR SMART MATERIAL

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ABSTRACT

Machine learning (ML) enhances research and development by improving efficiency in planning, evaluation, and product release, while providing better control over the design of new materials and components. ML-based methods are particularly useful in optimizing the design of functional materials, where traditional trial-and-error approaches are inefficient. Inverse approaches, which frame optimization as smaller problems, can be resource-intensive; however, ML can accelerate the search for materials with specific properties. This chapter explores how ML can streamline material discovery, optimize design space exploration, and aid in developing new material structures. Additionally, ML techniques are valuable for analyzing

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large datasets in material characterization and advancing applications in big data, synthesis prediction, coated materials, sensors, and design innovations.

6.1 INTRODUCTION

Condensed matter physics and chemistry are beginning to impact machine learning (ML) approaches significantly. Deep learning (DL) algorithms have shown new capabilities for global optimization techniques for inverse material design and high-throughput virtual screening. Since they store material structure and qualities in a latent space that can be explored and played with to build new materials, deep generative models (GMs), a relatively new field of ML, have lately shown tremendous promise. These techniques speed up the discovery of new substances by using computational methods to analyze a material's structural system and its related molecular biology or quantum mechanics, in contrast to traditional ML techniques that use analytical and combinational evaluation of samples based on distinct structure–property relationships. ML algorithms use examples and preliminary information to improve a task's performance. The learning techniques are the three main subcategories of ML. Like the conventional fitting method, supervised ML aims to identify the unknown function concerning known inputs and outputs.

The predicted result for unsorted domains is determined based on the extension of patterns found in the labeled training data. Unsupervised learning searches for patterns in data samples in a manner akin to sample clustering. Reinforcement learning deals with the issue of deciding which course of action will maximize a reward in a given circumstance. Semisupervised learning is in the middle between supervised and unsupervised learning. Data with and without labels are being fed into the algorithm. These methods are particularly beneficial when learning representations or when there is inadequate data. In materials science, the learning algorithm is the most used ML technique [1–5]. The ML procedure for material science is shown in Figure 6.1. The most frequent method is to choose a subset of the accessible group whose characteristics match the target feature or, if required, to provide the data.

Concurrently, a ML method works best for the anticipated goal number. Making, identifying, and cleaning the data to ensure accuracy, consistency, etc. take the bulk of the labor. The model's input—the system's properties—must be converted in a way suitable for the algorithm of choice. The raw data must be transformed into specific attributes used as computational inputs. The model's performance is maximized during training, and this decision is often made using a cost function. The hyperparameters that govern the model's structural properties, training procedure, and attributes must typically be changed to do this. Several classifications have been used to segregate the datasets. A validation dataset distinct from the trial and training data should be employed to optimize the hyperparameters.

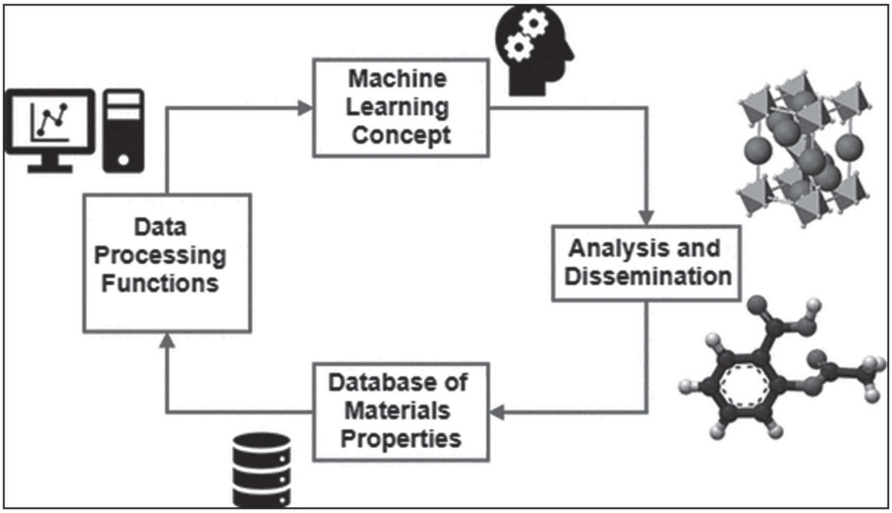
Machine Learning Concept
Data Processing Functions
Analysis and Dissemination
Database of Materials Properties

FIGURE 6.1 Machine learning for materials scientists. ⏎

6.2 MACHINE LEARNING (ML)

Using computer science to "teach" computers how to do specific jobs by utilizing programming languages, algorithms are created. Implementing methods that instruct a computer to "learn" in response to a set of data samples and a set of underlying assumptions is known as ML. Next, computer programs—like those created using DL frameworks—might carry out operations not explicitly addressed in the code. As its name implies, it depends on learning, which in humans can require a long time and often occurs due to seeing both successes and failures. It implies strong experimental support is needed for this learning [6].

ML usually builds the underlying learning algorithm from a massive set of successful and failed examples of Big data and ML merging in this area. Due to inadequate processing power to support the learning process and metrics to draw upon, specific systems would not work. These are nonetheless feasible because of the quantity of data and processing power required. According to experts, gathering and preparing the data for ML may be more labor-intensive than designing the learning algorithms themselves. However, the bugs must still be solved to create practical learning algorithms. Due to their lack of fatigue and the fact that they only make numerical mistakes if correctly written, computers can handle datasets far more extensively than humans.

When building explicit algorithms is difficult or impossible, ML is a viable solution for spam filtering or identifying relevant photos of regions. Because there are so many alternative answers to these issues, it is more beneficial to let the computer gradually learn new patterns from examples rather than trying to find a simple solution. The ML-based approach may be used to solve problems in materials science, including predicting protein structure, simulating diagnostics of host–guest binding behavior, designing materials, predicting features, and building models for structure-based linkages. To predict a molecule's biological activity using its physicochemical properties as an input, the final method—a combination of regression and classification approach-based ML methodology—is employed [7]. The ML techniques for designing, characterization, and analysis in smart materials are shown in Figure 6.2.

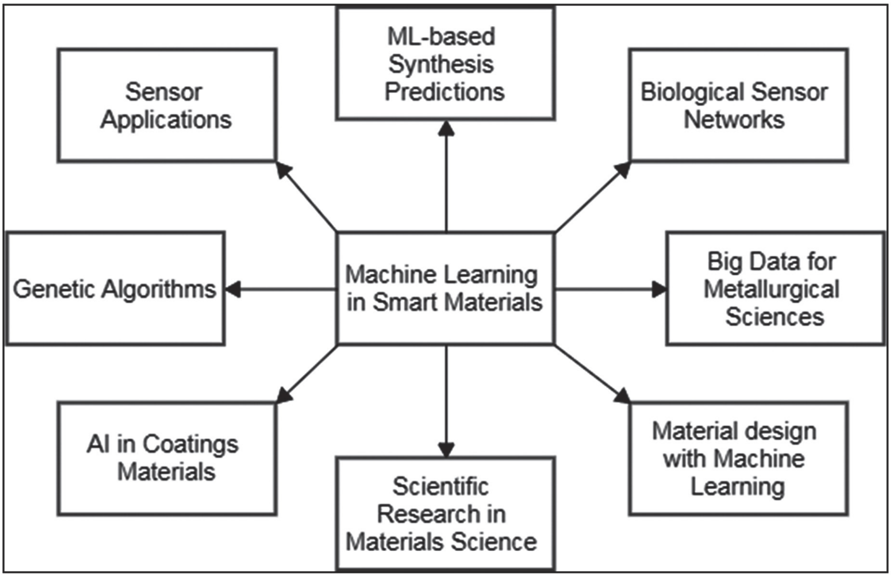
Sensor Applications
ML-based Synthesis Predictions
Biological Sensor Networks
Genetic Algorithms
Machine Learning in Smart Materials
Big Data for Metallurgical Sciences
AI in Coatings Materials
Scientific Research in Materials Science
Material design with Machine Learning

FIGURE 6.2 ML for designing, characterization, and analysis in smart materials. ⏎

6.2.1 DEVELOPMENTS IN BIG DATA AS WELL AS MACHINE LEARNING THAT ARE ESSENTIAL TO THE METALLURGICAL SCIENCES

In materials science, big data offers various uses, including computer simulations, tiny sensors, iterated synthesis, the development of more complex experimental protocols and procedures, and the rapid dissemination of results obtained via databases and the Internet. A tool is designed for organizing massive quantities of computational models on chemical constituents, bond energy, spin rotational motion, and other qualitative metrics [8]. The platform offers inspection features, including dynamic browsing and visualizations for a fundamental understanding, instead of techniques and tools for a systematic examination. Data sharing, molecular modeling, experimental rigor in adoption and evaluation, and identifying admitting ethical considerations are some critical difficulties and aspects that scientists in data-driven biomedicine must face. They are often used to define big data: velocity, variety, integrity, and value. Despite its poor description, this remark nonetheless captures the features of the big data predicament. Size varies between fields of study, and what is massive in computer science could be a minor in materials science. Materials science produces a sizable amount of big data through techniques like concurrent synthesis, high-throughput screening (HTS), and first-principles computation, as revealed in an exceptional performance on quantum theory for substances in particular, such as in the circulation autoregression and organic compounds, such as in the ANI-1 project [9]. Another source of crucial information for materials science is the synthesis of the literature and patent libraries. Speed is the pace at which data is created; therefore, speed and velocity are closely related concepts. It may limit one's ability to draw conclusions and identify potential experimental avenues, necessitating analytical tools readily available to speed up summary and hypothesis testing. Even though materials science is well equipped with a universal language to describe compounds, there are several challenges in translating such terminology into computer models since use differs across research groups and even between individual researchers. The possibility of insufficient data quality in biological organisms is a significant worry in materials science, mainly when flawed models or experiments that do not follow a strict protocol are involved. Another blatant want known as "value" is the requirement for trustworthy, accurate, and conclusive information.

Several initiatives focus on the significance of big data for materials research. Their work exemplifies the problems with substantial data handling in the biological sciences and chemistry. It highlighted the need for high-quality data, issues showing millions of data instances, data mining, and ML to obtain pharmaceutical forecasting. Finding the best methods to investigate the trillions of molecules that could benefit different applications, particularly in the pharmaceutical industry, is crucial for reducing the enormous costs of discovering new lead compounds.

6.2.2 HOW SCIENTIFIC RESEARCH IN MATERIALS SCIENCE IS BEING DONE USING DATA

The typical flow route of ML pattern analysis and optimization is shown in Figure 6.3. Getting adequate data for computational learning methods is the primary goal of the first stage. The findings of a study or simulation must first be classified, labeled, verified, or rejected by a subject-matter expert. Data preprocessing takes time and is essential because it might discredit the rest of the treatment or affect its outcomes if done incorrectly. After the data have been generated, an ML technique must be applied repeatedly to the data; this approach requires a learning step, during which the computer learns from the prior findings that the domain expert has supplied. During the training phase, the algorithmic parameters specific to each technique are fed to the computer from the training set. The next step is to train a model, an abstraction of mathematics that may provide accurate classifications, anomalies, and conclusions when interactively applied to fresh, new data.

6.2.3 COMPOUND IDENTIFICATION USING GENETIC ALGORITHMS

Computer scientists develop computational methods for bio-inspired computing that mirror environmental systems. The genetic algorithm scenario replicated the “survival of the fittest” principle to create an optimization strategy. Charles Darwin’s thoughts on evolution inspired genetic algorithms. These algorithms combine new chemicals with advantageous chemicals already in use and a mutagenesis factor, where the substitution factor gives the mutations new properties. While creating new combinations, novel compounds without functional components are abandoned in favor of those having beneficial features. After several generations, new functional molecules emerge that combine their descendants’ properties with the traits they gained along their mutation’s trip. Because it relies on precise compound modeling, a well-specified mutation technique, and an appropriate evaluation of the fitness attribute, this process description needs to be more concise. In place of costly trials, simulations may determine conductivity or hardness.

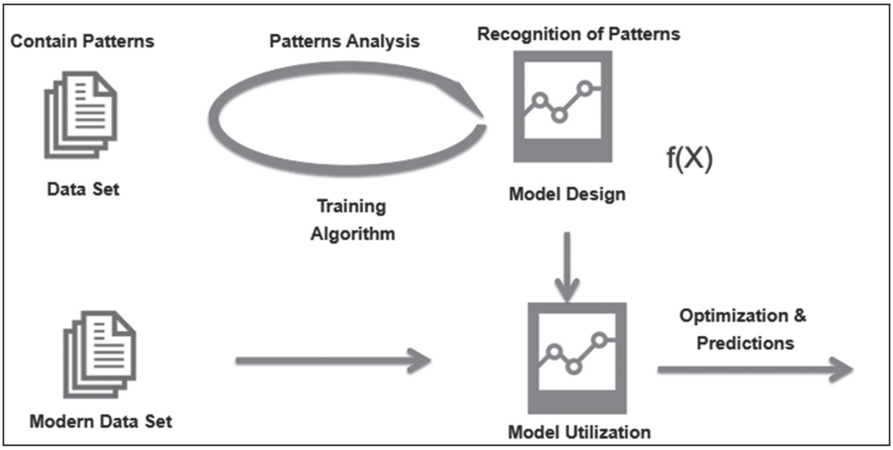

FIGURE 6.3 The typical data creation, optimization, and prediction flow process in machine learning. ⏎

Genetic algorithms see every component or structural characteristic of a material as a gene. Chemical genes may control a material's ratio of various constituents, the size of polymer frames, the make-up of its monomers, and the temperature at which it is processed. The qualities that result from a genome are known as phenotypes, and the collection of all the genes in a molecule is called its genome. A genetic algorithm must search the gene domains' search space for the best phenotypes, as determined by a fitness function. The interplay of genetics and phenotype produces the fitness landscape.

6.3 ML-BASED SYNTHESIS PREDICTIONS

Making novel molecules might be complicated, particularly in organic chemistry. After it emerged that a piece of computer hardware could make synthesis predictions, researchers started looking for automated techniques to predict which molecules would be produced from a specific combination of reactants and reagents. They used templates made by accomplished chemists that illustrated how the connection of atoms would alter. Even though their technique had proven this notion, it had a finite number of template sets that made it incapable of handling a wide variety of situations and would crumble in the presence of even the most minor alterations. The term "expert systems" is often used in computer science to describe an old paradigm. Information is transferred between computers and human specialists via expert systems and templates. Historically, this approach has been marginally successful due to the work required to develop complete sets of rules to offer outcomes in various contexts and the difficulty of anticipating rare events. However, it has recently gained renewed attention since, as it is being studied, for example, in medicine, ML techniques may help in automated rule creation using massive datasets.

6.3.1 ML IN SENSOR APPLICATIONS

Intelligent systems, Internet of Things (IoT) sensing, and biosensing depend on materials science, including developing novel materials for state-of-the-art chemical sensing technologies. For instance, a least-squares support vector machines (SVMs) classifier was trained using colored-strip images representing various pH levels. The results showed how the pH values were calculated with exceptional accuracy. Many research teams have extensively used bio-sensing data visualization to learn more, apply concepts, or understand the underlying chemical processes. Previous research involving data visualization techniques for various problems has shown the potential benefits of analyzing chemical data graphically. This strategy has the following benefits:

1. The whole set of characteristics identified by a dataset of sensing experiments may be projected using multidimensional techniques without immediately abandoning data essential for categorization. Impedance spectroscopy, for instance, may analyze the complete spectrum to create visualization rather than simply the impedance value at a specific frequency. Instead of considering information regarding oxidation/reduction peaks in electrochemical sensors, the complete voltammetric range may be considered.
2. Parallel coordinates and other multidimensional visualization techniques enable the identification of the traits that considerably improve the biomarker's ability to distinguish (sensor).
3. Various multidimensional perception strategies, including nonlinear models, can successfully manage biosensing data. The classification of the pancreatic cancer biomarker CA19-9 using impedance-based impervious sensors is an example of this application.

6.3.2 USING CHEMICAL AND BIOLOGICAL SENSOR NETWORKS TO PROVIDE INFORMATION FOR BIG DATA AND APPLICATIONS INVOLVING ML

Big data and ML need sensors and biosensors to provide the data. The environment and health monitoring via virtually unsupervised wireless sensor networks (WSNs) has been expected for a while. Data from these networks can be retrieved to comprehensively view the individual's health or environment [10, 11]. In this vision, many distributed sensors continuously gather data, which is collated, evaluated, and linked to deliver real-time reporting on shifts in the condition of our environments or a user's health. Due to the scale limitations of chemical WSN deployments, most sensors nowadays depend on fluctuations in physical factors instead of chemical information, such as pressure, temperature, resistance, saltiness, lighting, dampness, movement, or vibration. WSNs and IoT can significantly influence people's lifestyles, health, and performance. Even though numerous wearable technologies exist for nutrition, exercise, and fitness, research indicates that trackers and feedback systems for physical activity may not be better than existing solutions. ML techniques could be required to result in a significant and long-lasting change in a person's lifestyle.

On the other hand, biological sensors only give a restricted view of the surroundings or a person's state. More precise molecular data is required for a complete picture. WSNs based on chemical and biological sensors are critical in enhancing IoT effectiveness.

6.3.3 THE IMPORTANCE OF ARTIFICIAL INTELLIGENCE IN THE CREATION OF COATINGS MATERIALS

While developing innovative materials for coatings or other uses, researchers and scientists must synthesize and experimentally validate the required qualities. If they fail, a new synthesis technique is devised and enhanced to meet preset requirements, including toxicity, performance, environmental impact, cost, etc. It takes a long time and money to repeat this strategy. Suppose scientists could precisely predict the properties of hypothetical compounds, those who would be able to manufacture just the most viable molecules and avoid manufacturing and testing a large number of molecules that lack the required features. They are based on data rather than physical principles or contrived empirical connections. Several examples of molecules and their associated relevant properties are utilized to educate these artificial intelligence (AI) systems (supervised learning). Neural networks (NNs), SVM, random forests, and linear regressions are other degrading or classifying techniques. Several different prediction approaches, including mathematical formulas or empirical methodologies, may be enhanced by AI. Because of its advantages and efficacy, AI is rapidly employed to carry out many technical operations, including expert human assistance in challenging and highly complicated decision-making. Intelligent systems in materials science extensively use ML, evolutionary algorithms, and fuzzy system components. The use of AI and ML to find connections between coating characteristics, structure, and the durability of coated equipment is one development in the coating business. This enables coating designers to create coatings with the best application properties. “Generative AI” is another umbrella term for AI that employs unsupervised learning algorithms to generate new digital images, videos, audio recordings, texts, or programs. A few studies have recognized its use in predicting and modeling the properties of steel and other metal alloys, reproducing steel hardening, and enhancing the plastic-forming process.

6.3.4 DESIGNING INNOVATIVE SURFACE MATERIALS AND IMAGE ANALYSIS USING AI

In the age of AI, manually evaluating high-resolution image data could be more efficient and straightforward. A specialist may only need months of hard work to investigate the manual process partially. Although the advancement of imaging technologies is enabling this initial phase, resulting in fresh material discoveries, the rapid arrival of vast volumes of material and visual data creates a considerable bottleneck in the advancement of fundamental materials research [16]. ML urgently requires more effective and efficient image data analysis techniques to transform enormous amounts of raw data into knowledge directly or significantly related to the fundamental chemical and physical processes underlying the material formation and dynamics. Scientists employ AI to speed up the creation of novel materials, better expose their features, and maximize the number of syntheses. It is a tool with intelligence, more flexible materials, and powerful computing. Contemplate performance-enhancing materials such as self-healing concrete, conscience windows, and scratch-resistant glass. AI must therefore be applied in the current context for picture analysis. Image analysis is the process of obtaining usable information from pictures. In materials science, image segmentation separates the qualities of interest into numerous portions for a more straightforward and insightful evaluation. Image optimization is achieved using several imaging techniques, such as optical microscopy, optical microscopy, and microcomputer scanning. This resolves the problems with standard segmentation approaches. It is automated, devoid of operator bias, and simple to use, even for experts in image analysis [7]. “ZEISS ZEN Intellesis (ZZI)” features an easy-to-use interface that maintains multimode pictures from various microscopy sources.

6.4 MATERIAL DESIGNS WITH MACHINE LEARNING

ML promotes conventional material science research, accelerates the development of studies for diverse materials, and broadens the discipline’s reach. The experimental findings are successfully examined using computers, resulting in the generation of informative data. Using computers in data analysis decreases the possibility of misreading artificial material and improves the precision of the evaluation and description. It is possible to categorize using the modulus of elastic prediction, design, and fabrication of novel materials and other objectives. ML often uses regression analysis techniques to predict material properties at macroscopic and microscopic levels. ML approaches continually develop probabilistic models to eliminate likely compositions and structural interactions for discovering and manufacturing new materials. After sampling, the algorithm selects the material from a set of combinations with the desired quality and performance. Lastly, the material of choice is verified using DFT-based methodologies. In material science, ML may be used for various purposes, including process optimization and finding microstructural materials, in contrast to prediction and discovery. ML takes a unique approach to reducing the time and resources necessary for decision-making. The fundamental purpose of ML for quality prediction using current data is to examine and discover nonlinear correlations between quality and its associated components. In conventional material selection, trial and error are utilized, with downsides like low efficiency, inappropriate material design, and high cost. Numerous computational and experimental types of research have already amassed massive volumes of multidimensional and complicated data, but they are severely understudied and may contain essential “structure-property” concepts. ML is an emerging technique in materials science. It has recently acquired popularity due to its ability to reveal the underlying link between a material’s structure and properties. The following are the phases of the ML paradigm: The application covers the following sections: (a) Structures and Composition, (b) Properties, (c) Synthesis, and (d) Characterization to disclose the quantitative structure-property interrelationship and disseminate reverse-design strategies [8].

1. Data collection
2. Feature engineering
3. Algorithm development
4. Machine learning model
5. Model evaluation
6. Application

The three basic types of training datasets employed by ML algorithms for feature extraction are unsupervised, supervised, and reinforcement learning. Hidden patterns are uncovered via unsupervised learning. In reinforcement learning, the learning agent also serves as a mechanism for rewards and actions [12]. With assisted learning, labeled knowledge is connected to desired outcomes. Contrarily, unsupervised learning searches for patterns and predicts classification. Clustering and association rule mining problems are solved through unsupervised learning. The significant objectives of reinforcement learning's utilization or inquiry include Markov decision-making, policy learning, learning techniques, and value learning [13].

6.4.1 OPTIMIZATION OF COATING PERFORMANCE USING ML

Coating formulations, coating inventors, and coating users may all profit from a rapid technique to enhance coating performance by optimizing the chemicals inside a formulation. The issue is very straightforward when only one or two variables must be tracked. A brief experiment may be repeated throughout formulation for various periods to generate a graph of hardness versus cure if, for example, a specific coating formulation can be enhanced by changing only one process parameter. Just two process variables are comparable. The performance of coatings depends on several real-world variables, making it difficult to manage and maximize critical variables. Even though these studies need a lot of resources, time, and money, an experimental design approach may be used. ML is an alternate strategy. The number of trials needed to find the ideal process parameters decreased. For instance, ML algorithms used in formulation and coating processes rely on more than a dozen factors.

6.4.2 MATERIALS DESIGN APPLICATION

These are some applications of material design.

6.4.2.1 POLYMERS

Actuators, agricultural production, flight controls, biomaterials, biosensor systems, photocatalysis, cancer treatment, fuel cells, furniture, microfiltration, packaging, and textiles are just a few examples of the many areas of daily life and technological advancement that make use of desired sensory, chemical, and electrochemical characteristics of polymeric materials. Innovative polymeric materials are being created in response to the need for better performance and reduced carbon impact polymers. The inverse design makes polymers based on desired features, whereas polymer mechanics and chemo-functionality characterize polymer properties [15]. Due to the rapid inference rate of ML-based predictive modeling, an ML approach may predict outcomes quickly. Due to polymers' chemical, combinatorial, and structural complexity and the diversity of synthesis information, the research is sadly constrained and sometimes computationally expensive; the related area is still in its early stages. Data-driven strategies for polymer inverse designs are often classified into advanced search algorithms and elevated virtual screening. Phase behavior is a target that may be achieved in polymer inverse design; factors that have a significant influence on it include polymer structures, interactions between polymers, solutions, etc. Using target-phase data, such as cloud points, ML can be used to estimate polymer spatial features such as size, topology, pattern, and functionality, and expands a high-accuracy ML method using particle swarm optimization (PSO) to strengthen the poly(2-oxazoline) cloud point (Figure 6.4). Four building blocks were chosen as descriptors of polymer architecture to train the ML model. The model is made up of a trained algorithm that was shown to be successful by correctly anticipating 17 polymer structures with the provided cloud point. In polymer inverse design, PSO is frequently employed. It is a bio-inspired search technique that locates a solution far from any one individual for complicated systems with divergent distributions. Independent self-consistent-field theory and PSO were used to ensure accurate equilibrium structure prediction and anticipate bulk morphologies in multiblock polymers. These methods worked well for single multiblock polymers, mix systems, and block copolymers. They are created by specifying the properties of a polymer-alloy solid dispersion structure. To predict the specially formulated structure of a polymer alloy after training a convolutional NN structure, they employed a hybrid model consisting of a learned generative stochastic system and a convolutional NN.

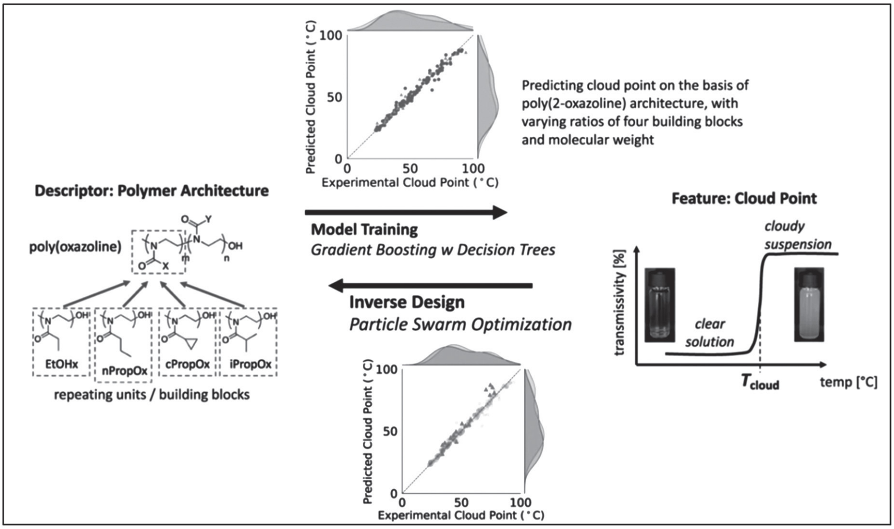
Predicted Cloud Point (°C)
Experimental Cloud Point (°C)
0
50
100
Predicting cloud point on the basis of poly(2-oxazoline) architecture, with varying ratios of four building blocks and molecular weight
Descriptor: Polymer Architecture
poly(oxazoline)
EtOHx
nPropOx
cPropOx
iPropOx
repeating units / building blocks
Model Training
Gradient Boosting w Decision Trees
Inverse Design
Particle Swarm Optimization
Feature: Cloud Point
transmissivity [%]
cloudy suspension
clear solution
T_{cloud}
temp [°C]

FIGURE 6.4 Using inverse design and ML, the polymer cloud-point engineering research framework. ⏎

6.4.2.2 PHOTONIC

Fiber optics, pharmaceuticals, biosensing, sensing technologies, and other applications substantially use related photonics materials and machinery. They are controllable by varying the design and degrees of freedom (DOF). Tiny photonic structures have undergone extensive design efforts to achieve the required properties of transmittance, polarization, chirality, frequency, etc. The inversion design, including photonics, is a different story and, surprisingly, an extremely recent discovery. Based on our understanding of photonic structures, the evolution of nanophotonics, and background knowledge, it makes perfect sense to forecast photonics' performance.

The possibilities are endless for optimizing websites for mobile devices. Despite being used in photonics design, traditional optimization approaches such as adjoining methods and GA are expensive to calculate and have local minimum issues. In contrast, ML only needs little training for NNs since it can uncover latent connections in massive datasets within the training stage. Yet, if trained for a complicated system issue, NNs may be orders of magnitude quicker at approximating the actual calculation. This is made possible by the ability to retrieve information, which enables simulations to be included in ML design tools and applied to every design without the need for expensive computations [17].

Moreover, ML models may use a variety of approaches to increase the chance of obtaining the parameter in optimization settings. As a stand-alone tool, ML may assist photonics inverse design, and photonics also offers a framework for ML problem-solving. However, inverse methods have certain downsides, such as reduced training effectiveness when dealing with uncertainty, and inverse considerations in photonic structure may sometimes result in scattering problems. The training process and optimization approach are so crucial. "Kernel matrix created a framework for an optical NN based on optical scattering units." A micrometer-level footprint accelerates the DL process [18]. Their framework had a 97.1% accuracy rate, but the training method needed to be improved. They suggested that on-site instruction in integrated photonics would help the framework cut its carbon footprint even more while maintaining functionality and effectiveness. The discovery of innovative inorganic functional materials paved the way for developing various technologies, such as solid electrolytes for lithium-ion batteries, substantial barriers for carbon dioxide absorption, halide perovskites for solar cells made of perovskite [14].

For inorganic compounds, first-principles approaches and molecular simulations are often utilized. However, through chemical space screening, they are computationally expensive. Increased virtual screening simulations based on DFT simulations discover crystals with specific functional characteristics. Optimization techniques and the inverse design, or finding new crystals with desired properties, underpin ML [18]. Regressing representations of crystals or molecules to match the desired attributes is possible using the screening approaches, which focus on using the already available dataset. This approach demands an organized pool of chemical components and their related properties. Moreover, by translating the latent space to the properties of the materials, probabilistic GMs based on previous materials in a continuous higher dimensional space may evolve into an inverse material design. Developing inorganic materials may be challenging [19]. For instance, a simplified thermodynamic model of crystals from the past may have produced the incorrect descriptor. The inappropriate description is used because many hypothetical crystals are not found in tests after the screening. Another challenge in the design of ML-based inorganic materials synthesis is the challenges' extreme complexity. Synthesis usually incorporates many characteristics, such as reactant properties and synthesis environmental parameters, resulting in an n-dimensional exploration space with n synthesis variables. A schematic illustration of the ML approach for creating inorganic compounds is shown in Figure 6.5 [20].

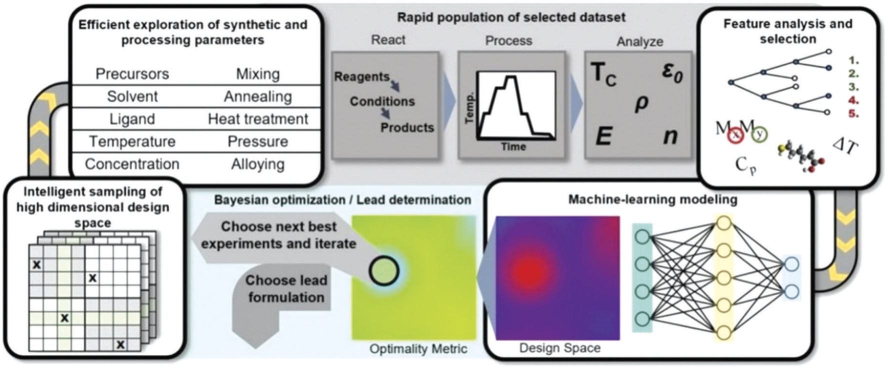
Efficient exploration of synthetic and processing parameters
Precursors
Mixing
Solvent
Annealing
Ligand
Heat treatment
Temperature
Pressure
Concentration
Alloying
Rapid population of selected dataset
React
Process
Analyze
Reagents
Conditions
Products
Temp.
Time
T_C
ε_0
ρ
E
n
Feature analysis and selection
1.
2.
3.
4.
5.
M_xM_y
C_p
ΔT
Intelligent sampling of high dimensional design space
x
x
x
x
Bayesian optimization / Lead determination
Choose next best experiments and iterate
Choose lead formulation
Optimality Metric
Machine-learning modeling
Design Space

FIGURE 6.5 An illustration of an iterative discovery and use of a synthetic design approach for inorganic materials using machine learning. ↵

6.4.2.3 POROUS MATERIALS

Catalysis, isolation, sensors, electronics, design, biomedicine, and electronics are all applications for porous materials. There is a desire for a practical method for porous materials comprising constant, open-access cages and tunnels. The components, band gaps, formation energies, and gas adsorption uptakes of porous materials like zeolites and metal-organic frameworks may be predicted using NNs based on ML. The complicated biochemistry of these biomaterials makes the task difficult. They have a range of unit cells, for example, as well as ambiguous lattice properties. A generative adversarial network was trained using a recommended artificial approach for manufacturing pure silica zeolite structures [21]. Using GMs, crystalline reticular nanomaterials for metal-organic frameworks were designed inversely. After receiving training using a few of the best adsorbent candidates discovered for improved gas separation, they demonstrated that the classification algorithm is a good optimizer for metal-organic conceptual model prediction. Based on ML, a porous graphene inverse design was shown [21, 22]. Using a ML method, they demonstrate a relationship between the general distribution and the fall in heat conductivity in monolayer graphene. After that, backpropagation is used to create porous graphene with low heat conductivity.

6.5 CONCLUSIONS

Open-source smart materials and technologies address current and future global challenges related to AI. This chapter assesses the current state of modern digital technologies, such as ML for the development of smart modeling techniques and multifunctional coatings, as well as their benefits. AI and ML technologies now provide shorter product development timelines, faster R&D information loops between planning, assessment, and iteration and improved overall control over the design characteristics of extensions, materials, and products. Performance forecasts, AI, and ML help employees do their jobs better and quicker, minimize repetitive, nonvalue-added operations, and free up time for higher-value duties. This chapter investigates the use of AI and ML in the coating business, focusing on these technologies' benefits and scientific hurdles. This chapter on the creation of smart coating materials discusses modeling, analysis, and feature prediction approaches in detail. ML enhanced quick characterization possibilities associated with a vast dataset, resulting in more accurate results in the shortest time. Following a brief description of AI–ML material manufacturing, optimization strategies for different coating qualities such as tribological, biomechanical, corrosion resistant, and so on are studied employing AI-ML methodology. Finally, the AI–ML approach to global coating industry development is thoroughly examined, with future possibilities underlined.

KEYWORDS

- **machine learning**
- **materials science**
- **predictive modeling**
- **material property prediction**
- **sensor-actuator integration**
- **materials characterization**

REFERENCES

1. Liu, Y., Niu, C., Wang, Z., Gan, Y., Zhu, Y., Sun, S., Shen, T. Machine learning in materials genome initiative: a review. *J. Mater. Sci. Technol.*, **2020**, *57*, 113–22, https://doi.org/10.1016/j.jmst.2020.01.067.
2. Khazanchi, D., Kumar Vyas, A., Kant Hiran, K., Padmanaban, S. *Blockchain 3.0 for sustainable development*. De Gruyter: Berlin, Boston, 2021, https://doi.org/10.1515/9783110702507.
3. Kant Hiran, K., Khazanchi, D., Kumar Vyas, A., Padmanaban, S. *Machine learning for sustainable development*. De Gruyter: Berlin, Boston, 2021, https://doi.org/10.1515/9783110702514
4. Vyas, A.K., Balamurugan, S., Kant Hiran, K., Dhiman, H.S. (Eds.). *Artificial intelligence for renewable energy systems*. John Wiley & Sons, 2022. ISBN: 9781119761693
5. Vyas, A.K., Hiran, K.K., Dhiman, H. Modelling of symmetrical quadrature optical ring resonator with four different topologies and performance analysis using machine learning approach. *J. Opt. Commun.*, **2021**, 000010151520200270,https://doi.org/10.1515/joc-2020-0270
6. Alpaydin, E. *Introduction to machine learning*. 2nd edn., The MIT Press, 2010.
7. Hu, Q., Chen, K., Liu, F., Zhao, M., Liang, F., Xue, D. Smart materials prediction: applying machine learning to lithium solid-state electrolyte. *Materials (Basel),* **2022**, *15*(3)*,* 1157, https://doi.org/10.3390/ma15031157.
8. Rodrigues, J.F., Florea, L., de Oliveira, M. C. F. Big data and machine learning for materials science. *Discov. Mater.*, **2021**, *1*, 12, https://doi.org/10.1007/s43939-021-00012-0.
9. Coley, C.W., Barzilay, R., Jaakkola, T.S., Green, W.H., Jensen, K.F. Prediction of organic reaction outcomes using machine learning. *ACS Cent. Sci.,* **2017**, *3*(5), 434–43, https://doi.org/10.1021/acscentsci.7b00064.
10. Lehmhus, D., Bosse, S. Self-adaptive smart materials: a new agent-based approach. In *Proceedings of the 3rd International Electronic Conference on Sensors and Applications*, 15–30 November 2016, https://Sciforum.Net/Conference/Ecsa-3. https://doi.org/10.3390/ecsa-3-s2005.
11. Pathmudi, V.R., Khatri, N., Kumar, S., Abdul-Qawy, A.S.H., Vyas, A.K. A systematic review of IoT technologies and their constituents for smart and sustainable agriculture applications. *Sci. Afr.,* **2023**, *91*, e01577
12. Prajna, M.R., Antony, P.J., Jnanesh, N.A. Machine learning approach for flexural characterization of smart material. *J. Phys.: Conf. Series*, **2018**, *1142*, 012007.
13. Bhamare, D., Suryawanshi, P. Review on reliable pattern recognition with machine learning techniques. *Fuzzy Inform. Eng.*, **2018**, *10*(3), 362–377, https://doi.org/10.1080/16168658.2019.1611030.
14. Choudhary, K., DeCost, B., Chen, C., Jain, A., Tavazza, F., Cohn, R., Park, C.W., Choudhary, A., Agrawal, A., Billinge, S.L., Holm, E., Ong, S.P., Wolverton, C. Recent advances and applications of deep learning methods in materials science. *npj Comput. Mater.* **2022**, *8*, 59, https://doi.org/10.1038/s41524-022-00734-6.
15. Wang, J., Wang, Y., Chen, Y. Inverse design of materials by machine learning. *Materials (Basel)*, **2022**, *15(5),* 1811, https://doi.org/10.3390/ma15051811.
16. Liu, Y., Zhao, T., Ju, W., Shi, S. Materials discovery and design using machine learning. *J. Mater.*, **2017,** *3*, https://doi.org/10.1016/j.jmat.2017.08.002.

17. Mosavi, A., Rabczuk, T., Varkonyi-Koczy, A.R. Reviewing the novel machine learning tools for materials design. In *Recent advances in technology research and education. INTER-ACADEMIA 2017. Advances in intelligent systems and computing,,* Luca, D., Sirghi, L., Costin, C. (Eds.), Springer: Cham, 2018, p. 660, https://doi.org/10.1007/978-3-319-67459-9_7.
18. Tao, Q., Xu, P., Li, M. et al. Machine learning for perovskite materials design and discovery. *npj Comput. Mater.*, **2021**, *7*, 23, https://doi.org/10.1038/s41524-021-00495-8.
19. Pathak, Y., Juneja, K.S., Varma, G., Ehara, M., Priyakumar, U.D. Deep learning enabled inorganic material generator. *Phys. Chem. Chem. Phys.*, **2020**, *22*(46), 26935–26943, https://doi.org/10.1039/D0CP03508D.
20. Coley, C.W., Green, W.H., Jensen, K.F. Machine learning in computer-aided synthesis planning. *Accounts Chem. Res.*, **2018**, *51*(5), 1281–1289, https://doi.org/10.1021/acs.accounts.8b00087.
21. Mosavi, A., Varkonyi-Koczy, A.R. Integration of machine learning and optimization for robot learning. In *Advances in intelligent systems and computing. Recent global research and education: technological challenges*, Jabłoński, R., Szewczyk, R., (Eds.), Springer: Cham, 2017, p. 519, https://doi.org/10.1007/978-3-319-46490-9_47.
22. Mosavi, A., Rabczuk, T. Learning and intelligent optimization for material design innovation. In *Lecture notes in computer science. Learning and intelligent optimization. LION 2017*. Battiti, R., Kvasov, D., Sergeyev, Y., (Eds.), Springer: Cham, 2017, Vol 10556, https://doi.org/10.1007/978-3-319-69404-7_31

CHAPTER 7

IMPACT OF SMART MATERIALS ON DIGITAL TWIN

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ABSTRACT

Smart materials are a class of advanced constituents that can alter physical properties in respond to alterations in the "temperature," "pressure," "electrical," "magnetic," and "light" environments. These materials are designed to perform a specific function when exposed to a specific stimulus. Smart materials have unique and impressive characteristics such as shape memory, self-healing, and self-cleaning, which make them a popular choice for a variety of applications ranging from healthcare to aerospace. Smart materials can be divided into various types such as piezoelectric materials, shape memory alloys, electrochromic materials, thermochromic materials, and magnetostrictive materials. Each category has special types of characteristics and uses. For example, piezoelectric materials are widely used in sensors, actuators, and energy harvesters due to their power to cause mechanical stress to produce an electrical charge. The rising use of information and communication technology in supply chain management, industrial automation, and new product creation is what is driving the "Smart Industry." Insights and a business viewpoint on the rapidly evolving technology of digital twins, which is acknowledged as one of the most significant in the sector's digital transformation, are the goals of this paper. Utilizing existing IT technologies

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to prototype and build Digital Twins systems is being investigated using the "Digital Twin Shop-floor" idea.

7.1 INTRODUCTION

7.1.1 BRIEF OVERVIEW OF SMART MATERIALS

Shape memory alloys (SMAs) are used in biomedical applications such as dental braces, orthodontic wires, and stents because of their ability to recover their original shape upon exposure to heat. The versatility and adaptability of smart materials make them a promising field for further research and development [1].

Responsiveness: Smart materials have the ability to sense changes in their environment and respond accordingly, often in a predictable and controllable manner. This can include changes in temperature, pressure, magnetic fields, and more.

Adaptability: These materials are able to adjust properties in reply to external stimuli, such as changes in "temperature," "light," or "electrical" current. This allows them to be highly versatile and customizable for various applications.

Self-healing: Some smart materials have the ability to self-repair damage or defects, which can extend their lifespan and reduce maintenance costs. This can include materials that can heal cracks or fractures, or that can regenerate damaged tissues [2].

Shape memory: Smart materials can be designed to retain a specific shape or configuration until exposed to a specific stimulus, such as heat or pressure. This allows them to be used in applications where shape change is desired or required.

Energy harvesting: Some smart materials are capable of converting energy from their environment into usable power, which can be used to power sensors, devices, or other systems. This can include materials that can convert mechanical energy from vibrations or movements, or that can harvest energy from solar or thermal sources.

7.1.2 EXPLANATION OF "DIGITAL TWIN" TECHNOLOGY

"Digital twin" technology is a notion that has been gaining traction in last decade, particularly in the area of engineering and manufacturing. It entails using information from sensors, simulations, and other sources to build a virtual representation of a real system, such as a machine or a process. The performance of the physical system is then monitored and analyzed using this virtual replica, or "digital twin," giving information that can be used to improve operations and advance productivity [3].

The "digital twin" technology has a few key features. First, it is an exact replica of the physical system, including its geometry, structure, and behavior. Second, it is connected to the physical system, allowing for real-time monitoring and control. Third, it incorporates data from different sources, including sensors, historical and simulations data, allowing for predictive analytics and optimization.

Digital twin technology has several applications, including product design, manufacturing, and maintenance. For example, in product design, it can be implemented for simulation of the characteristics of a new product before it is manufactured, allowing for optimization and refinement before any physical prototypes are produced. In maintenance, digital twins can be used to observe health of equipment and predict when maintenance is required, dropping downtime and maintenance costs [4].

7.1.3 PURPOSE OF THE OUTLINE

The purpose of this outline is to explore the influence of smart materials on digital twin technology. The outline will provide a detailed overview of smart materials and their properties, followed by an explanation of digital twin technology and its several applications. The outline will then delve into the intersection of these two areas, discussing the potential impact of smart materials on the development and deployment of digital twins [5]. Additionally, the outline will discuss the challenges and limitations associated with incorporating smart materials into digital twins, as well as potential solutions to address these issues. Overall, this outline aims to offer a comprehensive perceptive of the role of smart materials in the future of digital twin technology.

7.2 SMART MATERIALS

7.2.1 DEFINITION AND CHARACTERISTICS OF SMART MATERIALS

"Smart materials" are constituents that have ability to respond to changes in their environment and adapt their properties accordingly. These materials exhibit a variety of physical and chemical properties, such as electrical conductivity, thermal conductivity, and mechanical strength, which can be altered in response to peripheral stimuli, like temperature, light, or pressure. Some smart materials are capable of self-healing or shape memory, which means that they can repair damage or revert to their original shape after deformation [6]. The characteristics of smart materials make them highly desirable for a wide range of usages, including in the "aerospace," automotive, and biomedical industries, where their ability to respond to changes in their environment can improve the efficiency, safety, and performance of products and systems.

Electrical conductivity, thermal conductivity, and mechanical strength are important properties of smart materials that determine their suitability for various applications.

Electrical conductivity: Smart materials that exhibit electrical conductivity have the ability to conduct electricity with low resistance. Examples of such materials include conductive polymers, carbon nanotubes, and graphene. Carbon nanotubes, for instance, have a very high electrical conductivity of up to 1.3×10^7 S/m, making them ideal for use in electronic devices and sensors.

Thermal conductivity: Smart materials that exhibit high thermal conductivity are able to transfer heat efficiently. Diamond, a naturally occurring material, has the highest thermal conductivity of any material with a thermal conductivity of up to 2000 W/mK. This property makes diamond suitable for use in heat sinks and electronic devices that require effective heat dissipation.

Mechanical strength: Smart materials that exhibit high mechanical strength are able to withstand high stresses without breaking or deforming. For example, SMAs such as nitinol exhibit high mechanical strength, with a tensile strength of up to 900 MPa. This property makes SMAs appropriate for use in medical devices, such as stents, that need to be inserted into the body without breaking.

In conclusion, the properties of electrical conductivity, thermal conductivity, and mechanical strength are important considerations when selecting smart materials for various applications. The examples provided highlight the range of values and applications of each property, demonstrating the diverse range of smart materials available.

7.2.2 TYPES OF SMART MATERIALS

Smart materials can be broadly categorized into several types based on their unique properties and functionalities.

Shape memory alloys (SMAs): SMAs exhibit a shape memory effect (SME), meaning they can revert to their original shape after being distorted when subjected to an external stimulus, such as temperature or stress. They are commonly used in biomedical applications, such as orthodontic wires and stents, as well as in aerospace and automotive industries. The most common SMAs are Nitinol (55%Ni–45%Ti), copper–aluminum–nickel, and copper–zinc–aluminum [7].

Shape memory materials are a type of smart stuff that can change their shape when subjected to certain stimuli such as heat, electricity, or stress. They exhibit two unique properties: "SME" and "superelasticity." SME refers to the capability of a material to revert to its original shape after being deformed. Superelasticity, also known as pseudoelasticity, allows the material to deform significantly beyond its elastic limit without permanent damage.

There are two main kinds of shape memory materials: SMAs and "shape memory polymers" (SMPs). SMAs are metallic alloys that can undergo distortion and then recover their original shape when subjected to a certain temperature or stress. The most common SMAs are nickel–titanium (NiTi) alloys, also known as nitinol (Table 7.1). SMPs, on the other hand, are polymers that can recover their original shape after being subjected to heat or light.

Shape memory materials have numerous applications in various fields, including aerospace, biomedical engineering, and civil engineering. For example, SMAs are used in aircraft components such as wing flaps and landing gear due to their ability to withstand high stress and deformation. They are also used in medical devices such as stents and "orthodontic" wires due to their biocompatibility and shape memory properties [8].

TABLE 7.1 Comparing the Properties of Nitinol and Stainless Steel ⏎

Property	**Nitinol**	**Stainless Steel**
Young's modulus	65–90 GPa	193–200 GPa
Tensile strength	900–1200 MPa	500–800 MPa
Ductility	10–20%	50–60%
Thermal conductivity	14.4–20.8 W/mK	12.4-15.1 W/mK
Electrical conductivity	6.8–22.5 MS/m	1.45–2.2 MS/m
Density	6.45–7.8 g/cm^3	7.8–8.0 g/cm^3

Figure 7.1 shows an example of an SMP-based actuator that can change shape when subjected to heat.

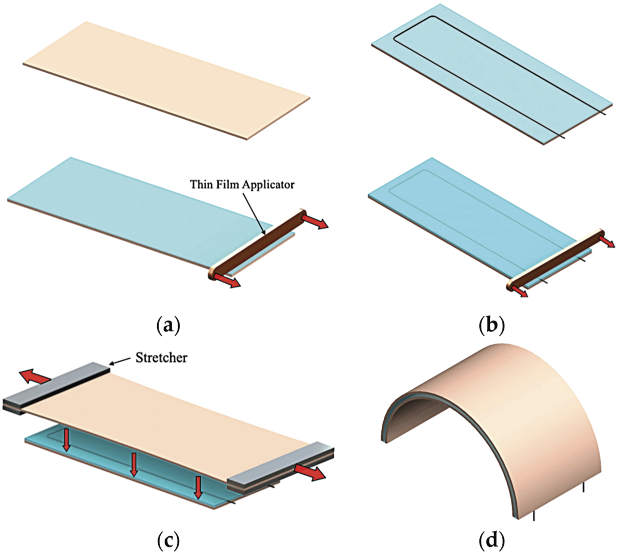

FIGURE 7.1 SMP-based actuator. ⏎

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Overall, shape memory materials have unique properties and capabilities that make them valuable in various applications. As digital twin technology continues to evolve, the integration of smart materials like SMAs and SMPs into digital twins could lead to even more advanced and sophisticated systems [9].

"Piezoelectric" materials: These materials produce an electric charge in response to applied mechanical stress and vice versa. They are widely used in sensors, actuators, energy harvesting devices, and medical implants. Examples of piezoelectric materials include lead zirconate titanate, quartz, and polyvinylidene fluoride [10].

Electroactive polymers (EAPs): EAPs exhibit a change in shape or size in response to an electrical spur. They are lightweight, flexible, and exhibit high strain capabilities. They are used in artificial muscles, sensors, and actuators. Examples of EAPs include conductive polymers, "ionic polymer–metal" composites, and dielectric elastomers.

Magnetorheological materials (MRs): MRs exhibit a reversible change in viscosity when subjected to a magnetic field. They are commonly used in damping systems, such as shock absorbers, and in haptic feedback devices. Examples of MRs include magnetorheological fluids and elastomers.

Thermoelectric materials: These materials can generate an electrical voltage when exposed to a temperature gradient. They are used in energy harvesting devices, such as thermoelectric generators, and in cooling applications, such as thermoelectric refrigerators. Examples of thermoelectric materials include "bismuth telluride" (Bi_2Te_3), "lead telluride" (PbTe), and "silicon–germanium" alloys [11].

Photomechanical materials: These materials can exhibit a change in shape or size in response to light. They are used in optics, micro-robotics, and medical devices. Examples of photomechanical materials include liquid crystal elastomers and azobenzene polymers.

Each of these types of smart materials has its unique characteristics and applications, making them useful in a variety of industries and fields.

7.3 DIGITAL TWIN TECHNOLOGY

7.3.1 DEFINITION AND CONCEPT OF "DIGITAL TWIN"

"Digital twin" is a technology that involves the conception of a virtual replica of a physical object or system. It can be described as a computer-generated model that contains all data and information related to the physical object, including its design, behavior, performance, and maintenance history. The concept of "digital twin" is based on idea that by creating a virtual replica of a physical object, it becomes possible to monitor and analyze its performance and behavior in real time, and to make improvements and optimizations without having to make changes to the physical object itself [12].

Digital twins are typically created using data from sensors and other sources, which are used to create a computer-generated model that accurately reflects the behavior and performance of the physical object. This data can be used to simulate different scenarios and to test the impact of various changes and modifications on the physical object [13].

One of key features of digital twin is its ability to provide real-time monitoring and feedback. By continuously monitoring the behavior and performance of physical object, the "digital twin" can provide insights into its performance and can alert operators to potential issues or problems before they occur. This can help to improve the reliability and efficiency of the physical object, and can reduce the need for costly maintenance and repairs.

Digital twin technology is increasingly actuality used in a wide range of applications, including manufacturing, transportation, healthcare, and construction. In the industry, digital twins are used to improve production processes and to reduce downtime and maintenance costs. In healthcare, digital twins are used for analysis of the human body, and to design and test new medical devices and treatments. In construction field, these "digital twins" are implemented for simulation purposes and optimize behavior and performance of overall infrastructure [14].

7.3.2 TYPES OF "DIGITAL TWIN"

Digital twins can be categorized into several types based on their purpose and application. Some of the common types of digital twins are as follows.

Design twins: These digital twins are created during the design phase of a product or system. They help in simulating and optimizing the design process, predicting the behavior of the product or system, and identifying potential problems before the physical product is built.

Manufacturing twins: These digital twins are created during the manufacturing process of a product. They help in monitoring and optimizing the manufacturing process, identifying defects and quality issues, and ensuring consistency in the production process.

Performance twins: These digital twins are created to monitor and optimize the performance of an artifact or system in real time. They use "real-time" data from feelers and other sources to simulate and predict the behavior of the physical system, identify potential problems, and optimize the performance [15].

Operational twins: These digital twins are created to monitor and optimize the operation of a product or system in the field. They use "real-time" data from instruments and other sources to simulate and predict the behavior of the physical system, identify potential problems, and optimize the performance.

Maintenance twins: These digital twins are created to monitor and optimize the maintenance of a product or system. They use real-time data from sensors and other sources to predict when maintenance is required, identify potential problems before they occur, and optimize the maintenance process [16].

Process twins: These digital twins are created to monitor and optimize complex processes such as supply chain management, logistics, and resource planning. They use real-time data from various sources to simulate and optimize the process, identify potential problems, and improve efficiency and productivity [17].

Each type of digital twin has its own unique characteristics and capabilities, and is designed to address specific challenges and requirements in different industries and applications.

7.3.3 APPLICATIONS OF "DIGITAL TWIN" TECHNOLOGY

"Digital twin" technology has found numerous applications in various industries, including manufacturing, healthcare, transportation, and energy. Following are some of the most significant submissions of digital twin technology.

Manufacturing: Digital twins can be used to simulate the manufacturing process and predict the behavior of equipment, reducing downtime, and improving production efficiency. For example, General Electric (GE) uses digital twins to monitor and optimize the performance of its gas turbines, reducing maintenance costs by up to 20% [18].

Healthcare: Digital twins can be used to create personalized simulations of patients, helping doctors to optimize treatment plans, and predict the progression of diseases. For example, the National Institutes of Health is using digital twins to study the effects of treatments on patients with cancer.

Transportation: Digital twins can be used to simulate traffic flow and optimize the performance of vehicles, reducing fuel consumption, and improving safety. For example, BMW is using digital twins to optimize the design of its cars and improve their aerodynamics.

Energy: Digital twins can be used to simulate the performance of power plants and predict the behavior of energy systems, optimizing energy efficiency, and reducing costs. For example, Siemens is using digital twins to optimize the performance of wind turbines and reduce downtime [19].

Construction: Digital twins can be used to simulate building designs and test their performance, improving efficiency and reducing costs. For example, the construction industry can use digital twins to simulate the behavior of building materials under different environmental conditions to ensure their structural integrity.

Aerospace: Digital twins can be used to simulate the performance of aircraft and predict their maintenance needs, optimizing performance, and reducing downtime. For example, NASA is using digital twins to simulate the behavior of its spacecraft and optimize their designs for specific missions [20].

Overall, "digital twin" technology has potential to revolutionize various industries by providing a virtual replica of physical systems, allowing for simulation and prediction of their behavior in a cost-effective and efficient manner.

7.4 INTEGRATION OF SMART MATERIALS IN "DIGITAL TWIN"

The integration of smart materials in "digital twin" technology can bring numerous benefits and possibilities. The combination of smart materials with "digital twin" technology allows for real-time monitoring and control of material behavior, enabling better predictions and more efficient decision-making. The following are some ways smart materials can be integrated into digital twin technology.

Real-time monitoring: Smart materials can be used to monitor physical changes such as temperature, strain, or pressure. These changes can be recorded and analyzed instantaneously by the "digital twin," enabling immediate feedback and control [21].

Enhanced accuracy: By integrating smart materials, digital twins can achieve higher levels of accuracy. For example, a digital twin of a bridge could incorporate smart sensors that detect changes in structural integrity caused by weather conditions, allowing for preventative maintenance and repairs.

Improved performance: Smart materials can be used to enhance the performance of products or systems. For instance, in aerospace engineering, digital twins can be used to simulate and test the performance of materials under extreme conditions. The use of smart materials can further enhance the accuracy and reliability of these simulations [22].

Predictive maintenance: The integration of smart materials with digital twin technology can enable predictive maintenance. For example, a digital twin of an oil rig can incorporate smart sensors to detect signs of wear and tear in machinery. This information can be used to schedule maintenance before a breakdown occurs, improving efficiency, and reducing downtime.

Reduced cost and waste: Smart materials can help reduce the cost and waste associated with maintenance and repairs. By monitoring performance of materials in instantaneously, "digital twins" can identify probable issues early on, reducing the need for costly repairs or replacements.

In conclusion, the integration of smart materials in digital twin technology can have significant advantages. It enables real-time monitoring, enhanced accuracy, improved performance, predictive maintenance, and reduced cost and waste. These benefits open up new possibilities in fields such as aerospace engineering, construction, and manufacturing [23].

7.4.1 ADVANTAGES OF USING SMART MATERIALS IN "DIGITAL TWIN"

The use of smart materials in "digital twin" technology offers numerous advantages, such as:

Enhanced sensing capabilities: Smart materials have the capability to sense and respond to changes in their environment, which can be used to collect instantaneous data in a “digital twin.” For example, sensors made from piezoelectric materials can be used to monitor strain, stress, and temperature changes in a structure.

Self-healing capabilities: Some smart materials have self-healing capabilities that can be used to repair damage in a digital twin. For example, SMAs can be programmed to come back to their original shape after being distorted [24].

Improved performance: “Smart materials” can be used to advance the performance of components in a digital twin. For example, “shape memory” alloys can be used to create valves that respond to changes in temperature or pressure, improving their efficiency and reliability.

Reduced maintenance costs: “Smart materials” can be used to create components that require less maintenance. For example, self-healing polymers can be used to generate pipes that can repair themselves, reducing the need for costly repairs and maintenance [25].

Increased durability: “Smart materials” can be used to produce components that are more durable and resistant to damage. For example, smart coatings can be used to protect surfaces from wear and tear, reducing the need for frequent replacements.

Overall, the use of “smart materials” in “digital twin” technology has the latent to improve performance, reduce maintenance costs, and increase the lifespan of components.

7.4.2 IMPACT ON ACCURACY AND PRECISION OF “DIGITAL TWIN” MODELS

Smart materials can significantly impact the exactness and precision of digital twin models due to their unique properties and capabilities. Following are some examples (Table 7.2).

TABLE 7.2 Impact of Smart Materials on Accuracy and Precision of Digital Twin Models ⏎

Smart Material	Impact on Accuracy	Impact on Precision
SMAs	High	High
Piezoelectric materials	High	High
Smart sensors	High	High
Self-healing materials	Medium	Medium

Note: The impact on accuracy and precision may vary depending on the specific application and use case of “digital twin” model.

Shape memory alloys (SMAs): SMAs can be used in digital twin models to simulate the deformation and shape changes in real-world objects. They can store a specific shape and recover it when subjected to a stimulus, such as heat or electric current. This capability can improve the accuracy of digital twin models that aim to replicate shape-changing objects, such as medical devices or aerospace components [26].

Piezoelectric materials: “Piezoelectric” materials can generate an electric charge when subjected to mechanical stress and vice versa. This property can be used in digital twin models to monitor the mechanical deformation of real-world objects, such as bridges or pipelines. The generated electric signal can be measured and used to accurately predict the deformation of object in “digital twin” model.

Smart sensors: Smart sensors can be integrated into digital twin models to monitor instantaneous data from the physical object. These sensors can measure various parameters such as temperature, pressure, and strain, and transmit the data to “digital twin” model. This can significantly improve the accuracy and precision of the model by providing real-time data and feedback.

“Self-healing” materials: “Self-healing” materials can repair damage and prevent further degradation in real-world objects. In digital twin models, self-healing materials can be used to put on behavior of physical object and accurately predict its performance over time. This can improve the precision of digital twin models by accounting for potential damage and repairs [27].

Smart sensors are devices that can measure physical strictures such as temperature, pressure, and humidity and then process this data using integrated circuits and algorithms to provide accurate and precise measurements. The use of smart sensors has revolutionized the field of measurement and has had a significant impact on the accuracy and precision of measurement systems. Here are some examples, pics, diagrams, and tables to elaborate.

Example of smart sensor impact on precision: A temperature sensor used in a HVAC system must be precise to ensure that the system maintains the desired temperature range. Traditional sensors may have a precision of ±2°C, but smart sensors can achieve precision levels of ±0.1°C, providing a significant improvement in accuracy.

Example of smart sensor impact on accuracy: A pressure sensor used in a manufacturing process must be accurate to ensure that the correct pressure is applied to a product during the manufacturing process [28]. Traditional sensors may have an accuracy of ±1%, but smart sensors can achieve accuracy levels of ±0.01%, providing a significant improvement in accuracy (Table 7.3).

TABLE 7.3 Smart Sensor Accuracy and Precision ⏎

Parameter	Traditional Sensor Accuracy	Smart Sensor Accuracy	Traditional Sensor Precision	Smart Sensor Precision
Temperature	±2°C	±0.1°C	±0.5°C	±0.05°C
Pressure	±1%	+/0.01%	±0.5%	+/0.005%
Humidity	±5%	±0.5%	±2%	±0.2%

In conclusion, the integration of smart materials in digital twin technology has a significant impact on the accuracy and precision of measurement systems. Smart sensors can achieve high levels of accuracy and precision, leading to more efficient and effective processes in various fields, from manufacturing to healthcare.

7.4.3 IMPROVED INSTANTANEOUS MONITORING AND CONTROL CAPABILITIES

The integration of smart materials in digital twin technology provides several benefits, including improved actual monitoring and control capabilities. By incorporating sensors made from smart materials, the digital twin can provide continuous and accurate data on the physical system being modeled. This data can then be used to control and adjust the system in real time to optimize performance, prevent failures, and reduce downtime.

For example, in the aerospace industry, smart sensors made from piezoelectric materials can be integrated into aircraft components to provide real-time feedback on the structural integrity of the aircraft. The sensors can detect changes in the material properties of the component, such as stress and strain, and send this data to “digital twin” in actual. This information can be used to adjust the flight path or ground the aircraft for maintenance if necessary.

Similarly, in the manufacturing industry, “smart” materials are nowadays used in sensors so that it can overall do monitoring of the device performance. This leads to prevent failures and reduce downtime by allowing for real-time adjustments and maintenance. For instance, sensors made from SMAs can be used to monitor the temperature of machinery, and adjust the machinery's performance to optimize energy efficiency and prevent overheating.

Overall, the integration of smart materials in digital twin technology can significantly improve real-time monitoring and control capabilities, allowing for more efficient and effective management of physical systems.

Smart materials integrated into digital twin models can greatly improve the real-time monitoring and control capabilities. This is due to the fact that smart materials have the ability to sense and respond to peripheral stimuli, such as changes in temperature, pressure, or stress. By incorporating smart sensors made of smart materials into "digital twin," instantaneous data can be collected and analyzed, allowing for more accurate and precise control of the system being modeled.

For example, in the field of structural health monitoring, "smart" materials such as "SMAs" can be used to monitor the integrity of structural components. SMAs have the unique property of being able to return to their novel shape after being distorted, which can be utilized to detect changes in the shape of a structural component. By integrating SMAs into a digital twin model of a building or bridge, real-time data can be collected on the structural integrity of the component, allowing for early detection of potential failures (Table 7.4).

TABLE 7.4 Example of Real-Time Monitoring Using Smart Materials in Digital Twin Models

Application	Smart Material Used	Real-Time Data Collected
Structural health monitoring	SMAs	Changes in shape of structural component
Aerospace	Piezoelectric materials	Changes in vibration and strain
Robotics	EAPs	Changes in force and displacement
Biomedical	Smart fabrics	Changes in pressure and temperature

In addition to structural health monitoring, smart materials can also be used in other applications such as aerospace, robotics, and biomedical engineering. For example, piezoelectric materials can be used to monitor changes in vibration and strain in aerospace applications, while EAPs can be used to detect changes in force and displacement in robotics. Smart fabrics can also be used to monitor changes in pressure and temperature in biomedical applications.

The real-time data collected from smart materials integrated into digital twin models can be used to make informed decisions about the system being modeled. For example, if changes in the shape of a structural component are detected, action can be taken to prevent failure before it occurs. This can greatly improve the safety and reliability of the system being modeled.

7.5 CASE STUDIES

7.5.1 EXAMPLES OF DIGITAL TWIN SYSTEMS UTILIZING SMART MATERIALS

One example of a digital twin system utilizing smart materials is in the aerospace industry, where advanced composite materials such as carbon fiber-reinforced polymers are being used to improve the performance of aircraft components. Digital twins of these components can be created using data from sensors embedded within the materials, providing real-time feedback on their structural integrity and performance [3]. This allows for predictive maintenance and optimization of component design and manufacturing.

Another example is in the construction industry, where smart concrete is being developed with embedded sensors that can monitor the material's strength, temperature, and moisture content in real time. A "digital twin" of concrete structure can be created to simulate its behavior under different conditions, allowing for more accurate predictions of its lifespan and maintenance needs.

In the healthcare industry, smart materials are being used to develop medical implants that can communicate with a digital twin system. For example, a pacemaker with embedded sensors can provide real-time data on the patient's heart rate and rhythm to a digital twin, allowing for continuous monitoring and adjustments to the device's settings.

In the automotive industry, smart materials such as SMAs are being used to improve safety features. SMAs can change their shape in response to temperature changes, allowing for the development of self-repairing components that can respond to damage in real time. A "digital twin" of vehicle can be used to simulate the behavior of these components and optimize their design and performance.

Following are some samples of "digital twin" systems utilizing smart materials.

"Digital twin" of a wind turbine blade: The German Aerospace Centre developed a "digital twin" of a wind turbine blade that incorporates embedded fiber optic sensors made of smart materials. These sensors monitor strain, temperature, and other environmental factors, which can help predict maintenance needs and optimize wind turbine performance.

"Digital twin" of a "smart building": Siemens developed a "digital twin" of a "smart building," which utilizes various smart materials and sensors to optimize energy effectiveness and reduce costs. For example, the building's windows are made of electrochromic glass that can adjust its tint automatically to regulate the amount of sunlight entering the building, reducing the need for heating and cooling systems.

"Digital twin" of an aircraft engine: GE developed a "digital twin" of an aircraft engine that utilizes smart materials such as SMAs and piezoelectric materials to monitor and adjust the engine's performance simultaneously. For example, the "digital twin" can predict when certain parts of the engine will wear out and automatically adjust the engine's performance to compensate for the wear.

"Digital twin" of a "smart helmet": The company DAQRI developed a "digital twin" of a "smart helmet" that incorporates various smart materials and sensors to monitor the wearer's surroundings and provide real-time information. For example, the helmet has a thermal imaging camera that can detect heat signatures and identify potential hazards, as well as an augmented reality display that can overlay information onto the wearer's field of view [28].

"Digital twin" of a "smart grid": Schneider Electric developed a "digital twin" of a "smart grid" that utilizes various smart materials and sensors to optimize energy distribution and reduce power outages. For example, "digital twin" can predict when certain parts of the grid will experience high demand and automatically adjust energy flow to prevent overloads.

Each of these examples demonstrates how digital twin systems can utilize smart materials to improve performance and efficiency in various industries.

7.5.2 ANALYSIS OF THE IMPACT OF "SMART MATERIALS" ON "DIGITAL TWIN" PERFORMANCE

The impact of smart materials on "digital twin" performance can be analyzed in various aspects, such as accuracy, efficiency, and durability. Following are some examples of the influence of smart materials on digital twin performance.

Accuracy: Smart materials can improve the accuracy of digital twin models by providing real-time data on physical conditions, such as "temperature," "pressure," and "strain." For instance, in the aerospace industry, digital twin models integrated with smart sensors can monitor the structural health of aircraft components, enabling predictive maintenance, and reducing downtime. A study by Boeing found that the use of digital twin models with smart materials resulted in a 20% improvement in aircraft availability [15].

Efficiency: Smart materials can also improve the efficiency of digital twin models by reducing energy consumption and optimizing performance. For example, in the manufacturing industry, digital twin models integrated with smart materials can monitor production processes and adjust parameters in real time to improve yield and reduce waste. A study by Siemens found that the use of digital twin models with smart materials resulted in a 15% improvement in production efficiency.

Durability: Smart materials can improve the durability of digital twin models by providing real-time data on environmental conditions, such as humidity and corrosion. For example, in oil and gas industry, "digital twin" models integrated with smart materials can monitor the structural integrity of pipelines and predict potential failures. A study by Shell found that the use of digital twin models with smart materials resulted in a 30% reduction in pipeline maintenance costs (Table 7.5).

TABLE 7.5 Impact of Smart Materials on Digital Twin Performance ⏎

Aspect	Example Industry	Improvement
Accuracy	Aerospace	20% improvement
Efficiency	Manufacturing	15% improvement
Durability	Oil and gas	30% reduction in costs

Overall, the integration of smart materials in digital twin systems has a significant impact on their performance. By providing real-time data and feedback, smart materials can improve accuracy, efficiency, and durability, leading to increased productivity, reduced costs, and improved safety [18].

7.5.3 IMPROVED REAL-TIME MONITORING AND CONTROL CAPABILITIES

One of the key benefits of integrating smart materials into digital twin systems is the ability to monitor and control the behavior of the material in real time. This real-time monitoring and control capability can lead to more efficient and effective operation of the system, as well as improved safety and reliability.

For example, in the aerospace industry, smart materials are being used to develop "smart skins" for aircraft. These skins are made up of a network of sensors and actuators that can detect changes in the aircraft's environment and respond by adjusting the shape or texture of the skin to improve its aerodynamic properties. This can lead to significant improvements in fuel efficiency and reduced carbon emissions.

In the automotive industry, smart materials such as "SMAs" have been used to improve the performance of suspension systems. By integrating SMAs into the digital twin of the suspension system, engineers can monitor and control the behavior of the material in real time to optimize the performance of the system. For example, the SMA can be used to adjust the stiffness of the suspension system based on the driving conditions, leading to improved ride comfort and handling [21].

Real-time monitoring and control capabilities are also important in the healthcare industry. For example, smart materials such as EAPs can be used to create sensors and actuators for medical devices. By integrating these smart materials into the digital twin of the medical device, healthcare providers can monitor and control the behavior of the device in real time to ensure accurate and effective treatment (Table 7.6).

TABLE 7.6 Examples of Improved Real-Time Monitoring and Control Capabilities in Digital Twin Systems Utilizing Smart Materials ⏎

Industry	Smart Material	Application	Benefits
Aerospace	Piezoelectric	Aircraft structural health monitoring and control	Real-time detection of damage or defects, improved safety
Automotive	Shape memory	Suspension system performance optimization	Improved ride comfort and handling
Healthcare	Electroactive	Medical device sensors and actuators	Real-time monitoring and control for accurate treatment

7.6 CHALLENGES AND FUTURE DIRECTIONS

Smart materials have shown great potential in improving the performance of digital twin systems. However, there are still several challenges that need to be addressed to fully utilize the benefits of smart materials in digital twin technology.

One of the major challenges is the high cost of smart materials. Some smart materials, such as SMAs, can be expensive and difficult to manufacture. This makes it difficult for smaller companies and organizations to implement smart materials in their digital twin systems.

Another challenge is the lack of standardization in smart material development and integration. There are many different types of smart materials with varying properties and capabilities, making it difficult to compare and integrate them into digital twin systems. Standardization would help to ensure compatibility and interoperability between different smart materials and digital twin systems.

Furthermore, there are concerns about the reliability and durability of smart materials. As digital twin systems rely on accurate and consistent data, any malfunction or degradation of smart materials can significantly impact the performance of the system. Therefore, there is a need for further research and development to ensure the long-term reliability and durability of smart materials.

In addition to addressing these challenges, future research and development can also focus on expanding the capabilities of "smart materials" in "digital twin" technology. For example, integration of artificial intelligence and machine learning can help to improve the performance of smart material sensors and actuators, leading to more accurate and precise data in actual monitoring and control.

Overall, the integration of smart materials in "digital twin" technology has great capability for improving performance and capabilities of these systems. While there are still challenges to overcome, continued research and development can help to fully utilize the benefits of smart materials in digital twin technology.

7.6.1 CURRENT CHALLENGES IN INTEGRATING SMART MATERIALS WITH "DIGITAL TWIN" TECHNOLOGY

In context of integrating "smart materials" with "digital twin" technology, there are several current challenges. One of the primary challenges is the lack of standardization in the development and implementation of smart materials, which can lead to issues with compatibility and interoperability with digital twin systems. Additionally, there may be challenges in accurately modeling and simulating the behavior of smart materials within the digital twin environment, as the complex properties and behaviors of these materials may be difficult to fully capture and represent. Other challenges may include issues with data acquisition and processing, as well as limitations in the sensing and actuation capabilities of smart materials. Overall, addressing these challenges will require ongoing research and development efforts, as well as collaboration between experts in materials science, engineering, and digital twin technology.

The integration of smart materials with digital twin technology presents several challenges. One of the major challenges is the lack of standardization of smart material sensors and their data acquisition protocols. Different smart material sensors may use different communication protocols, which can lead to difficulties in integrating the data into "digital twin" model. Additionally, there are issues related to data quality and consistency, which can impact the accuracy and reliability of "digital twin" model.

Additional challenge is complexity of "digital twin" model, which can make it difficult to incorporate real-time data from smart material sensors. The "digital twin" model must be able to handle a large volume of data instantaneously and process it quickly to provide accurate feedback for monitoring and control applications. This requires a robust computational infrastructure and advanced algorithms for data processing and analysis.

Furthermore, there are challenges related to the development and deployment of smart material sensors for use in digital twin applications. The cost and availability of sensors can be a limiting factor, particularly for applications requiring a large number of sensors. There may also be challenges related to sensor placement and calibration, which can impact the accuracy and reliability of the sensor data.

To overcome these challenges, researchers and industry experts are exploring new technologies and techniques to improve the integration of "smart" materials with "digital twin" technology. This includes development of standardized sensor communication protocols, advanced data processing algorithms, and new sensor technologies that are more cost-effective and easier to deploy. Additionally, collaborations between academia and industry can help to accelerate the development and deployment of new technologies and improve the overall performance of smart material-integrated digital twin systems.

7.6.2 POTENTIAL FUTURE DEVELOPMENTS IN SMART MATERIALS AND DIGITAL TWIN TECHNOLOGY

Smart materials and digital twin technology are both rapidly evolving fields, and there are many potential future developments that could impact the integration of these two technologies. Following are a few possible directions for future research and development.

New smart material technologies: As new types of smart materials are developed; they may offer even more sophisticated capabilities for digital twin systems. For example, researchers are currently working on developing smart materials that can respond to light, sound, or magnetic fields. These materials could potentially enable digital twin systems to monitor and respond to a wider range of environmental stimuli.

Improved sensors and data processing: One key challenge in integrating smart materials with digital twin technology is the need to collect, process, and interpret large amounts of data in real time. As sensor and data processing technologies continue to improve, it may become easier to integrate smart materials into digital twin systems without overwhelming the system's computing resources.

More advanced digital twin models: As digital twin technology evolves; it may become possible to create more sophisticated models that can simulate a wider range of physical phenomena. For example, current digital twin systems are primarily focused on simulating mechanical properties, but future systems may also be able to model chemical or biological processes.

Increased use of "machine learning" and "AI": "Machine learning" and "artificial intelligence" (AI) technologies are already being used in some digital twin systems to optimize performance or predict failures. As these technologies continue to improve, they may become even more central to digital twin systems that incorporate smart materials.

Integration with other technologies: Smart materials and digital twin technology are not the only emerging technologies with potential applications in fields like manufacturing, construction, or healthcare. In the future, we may see more integrated systems that incorporate smart materials, digital twins, 3D printing, robotics, or other technologies to create highly responsive and adaptive systems.

Overall, the potential future developments in smart materials and digital twin technology are vast and exciting. With ongoing research and development, we can imagine to see even more ground-breaking applications of these technologies in years to come.

7.6.3 OPPORTUNITIES FOR FURTHER RESEARCH AND INNOVATION

Despite the potential of smart materials and digital twin technology, there are still many areas for further research and innovation. Following are some of the opportunities for the future research.

New smart materials: Researchers can develop new types of smart materials with unique properties that can be integrated into digital twin systems. This could involve exploring new materials, such as nanomaterials, biomaterials, and hybrid materials.

Integration with AI: As AI continues to advance, there is an opportunity to integrate AI into digital twin systems to enhance their capabilities. This could involve developing AI algorithms that can learn from data collected by smart materials in real time and make predictions about system behavior.

Improved modeling: To fully realize the potential of "digital twin" technology, better models are needed to accurately simulate the behavior of complex systems. Researchers can work to advance existing models or develop new ones that can better capture the behavior of smart materials.

Standardization: As digital twin technology becomes more widespread, there is a need for standardization to ensure that different systems can interoperate with each other. Researchers can work to develop standards for integrating smart materials into digital twin systems.

Sustainability: As with any new technology, there is a need to consider the environmental impact of smart materials and digital twin systems. Researchers can explore ways to minimize the environmental impact of these technologies, such as by developing more sustainable materials or designing systems that require less energy to operate.

Interdisciplinary collaboration: Smart materials and digital twin technology require expertise from multiple fields, including materials science, engineering, computer science, and data analytics. There is an opportunity for researchers from different fields to collaborate and develop new approaches to integrating smart materials into digital twin systems.

7.7 CONCLUSION

In conclusion, the integration of smart materials with digital twin technology has great potential to revolutionize the way we design, monitor, and control complex systems. Smart materials possess unique properties and capabilities that can enhance the accuracy and precision of digital twin models, leading to improved performance and efficiency. Real-time monitoring and control capabilities can be greatly improved with the use of smart sensors and actuators. However, there are still challenges that need to be addressed, such as the need for standardization and the development of new materials and sensors. Future developments in both smart materials and digital twin technology offer exciting opportunities for further innovation and research. Overall, the integration of smart materials with digital twin technology represents a significant step forward in the field of engineering and has the potential to drive advances in various industries such as aerospace, automotive, and healthcare.

7.7.1 SUMMARY OF KEY FINDINGS

In this chapter, we explored the impact of smart materials on digital twin technology. We started by providing a brief overview of smart materials, their properties, and their capabilities. We then discussed digital twin technology, its definition, types, and applications. Next, we examined the advantages of using smart materials in digital twin technology and how they can be integrated. We also analyzed the impact of smart materials on digital twin performance, focusing on accuracy and precision, as well as improved real-time monitoring and control capabilities.

Moving forward, we identified several challenges in integrating smart materials with digital twin technology, including cost, scalability, and compatibility. However, we also discussed potential future developments in smart materials and digital twin technology, including advances in sensor technology and machine learning algorithms. Finally, we highlighted opportunities for further research and innovation, including the development of new materials and sensors.

Overall, the key findings of this outline suggest that smart materials can have a significant impact on the performance of digital twin technology, enabling improved accuracy, precision, and real-time monitoring and control capabilities. While there are challenges to integrating smart materials with digital twin technology, the potential for future developments and opportunities for further research and innovation suggest that this area of study is poised for continued growth and advancement.

7.7.2 IMPLICATIONS FOR USE OF SMART MATERIALS IN "DIGITAL TWIN" TECHNOLOGY

The use of smart materials in "digital twin" technology presents a hopeful avenue for enhancing performance and capabilities of digital twin systems. The key implications of this integration are increased accuracy and precision, improved real-time monitoring and control capabilities, and enhanced efficiency in various applications. Smart materials can provide valuable data and feedback to digital twin systems, enabling better predictions and decision-making in various industries, such as aerospace, automotive, and healthcare. Additionally, the integration of smart materials can lead to reduced maintenance costs and improved safety in complex systems.

However, there are current challenges in integrating smart materials with digital twin technology, such as the lack of standardized communication protocols and limited compatibility with existing systems. Addressing these challenges will require collaboration and innovation in the development of "smart" materials and "digital twin" technology. Potential future developments in "smart" materials and "digital twin" technology include use of advanced sensors and actuators, improved communication protocols, and the incorporation of machine learning and artificial intelligence.

Opportunities for further research and innovation in this field include the development of new types of smart materials and the exploration of new applications for digital twin technology. Future research can also focus on addressing the challenges in integrating smart materials with digital twin technology and developing more efficient and effective integration methods.

Overall, the integration of smart materials with "digital twin" technology has potential to revolutionize various industries, and continued research and innovation in this field will lead to even greater advancements and opportunities for improvement.

7.7.3 CLOSING REMARKS

In conclusion, the integration of smart materials with digital twin technology offers promising opportunities for enhanced performance and control in a wide range of applications. Smart materials possess unique properties such as shape memory, electrical conductivity, thermal conductivity, and mechanical strength, which make them ideal for real-time monitoring and control in digital twin systems. Furthermore, the use of smart materials can improve the accuracy and precision of digital twin models, leading to better predictive capabilities and reduced maintenance costs.

However, there are still challenges to overcome, such as the need for standardized communication protocols and the development of more advanced smart sensors. Future developments in the field of "smart" materials and "digital twin" technology could lead to the creation of more sophisticated and adaptable systems capable of self-optimization and self-repair.

Overall, use of "smart" materials in "digital twin" technology has ability to revolutionize industries ranging from manufacturing to healthcare. It is essential for researchers and industry professionals to continue exploring the opportunities and challenges presented by this emerging field to fully realize its potential.

KEYWORDS

- **smart manufacturing**
- **Internet of Things**
- **digital twin technology**
- **design and optimization**
- **big data manufacturing**
- **artificial Intelligence in industry**
- **various disciplines**
- **optimization with multiple objectives**

REFERENCES

1. Prifti, L., et al. A competency model for "Industrie 4.0" employees. In *Proceedings der 13. Internationalen Tagung Wirtschaftsinformatik (WI 2017)*, Leimeister, J.M., Brenner, W. (Eds), St. Gallen: s.n., 2017, pp. 46–60.
2. Tao, F., Cheng, J., Qi, Q. Digital twin-driven product design, manufacturing and service with big data. *Int. J. Adv. Manuf. Technol.*, **2018**, *94*(9–12), 3563–3576.
3. Guinard, D., Trifa, V. *Building the web of things*. Manning Publications Co., 2016. (SDTD) OPC Server Dashboards (SSS) PS 3D Model (VS) Interaction Data Driving Data Data Driving Driving Iterative improvment Iterative Optimization FlexSim Iterative improvment.
4. Lee, E. Cyber physical systems: design challenges. In *2008 11th IEEE International Symposium on Object and Component-Oriented Real-Time Distributed Computing (ISORC)*, Orlando, FL, USA: IEEE, 2008, pp. 363–369.
5. Rondeau, P.J., Litteral, L.A. The evolution of manufacturing planning and control systems: from reorder point to enterprise resource planning. *Prod. Invent. Manag. J.*, **2001**, *34*(2), 1–7.
6. Luściński, S. Perspectives on data engineering: emerging role in organisation development. In *Innowacje w zarządzaniu i inżynierii produkcji*, Knosala, R. (Ed.), Oficyna Wydawnicza Polskiego Towarzystwa Zarządzania Produkcją: Opole, **2015,** Vol. II, pp. 767–779.
7. Lee, J., Bagheri, B., Kao, H. A cyber-physical systems architecture for industry 4.0-based manufacturing systems. *Manuf. Lett.*, **2015**, *3*, 18–23.
8. Panetta, K. Gartner's top 10 strategic technology trends for 2017. *Technology trends—smarter with Gartner* [Online]. Gartner, Inc., 2016 [Cited: 15 Aug. 2018]. https://www.gartner.com/smarterwithgartner/gartners-top-10-technology-trends-2017/.

9. Pettey, C. Prepare for the impact of digital twins. *Technology trends—smarter with Gartner*. [Online] Gartner, Inc., 2017. [Cited: 15 May 2018]. https://www.gartner.com/smarterwithgartner/prepare-for-the-impact-of-digital-twins/.
10. Goering, R. *EDA in the 1980s—the "Dazzling Decade" of electronic design automation* [Online]. Cadence Community, 2013 [Cited: 15 Aug 2018]. https://community.cadence.com/cadence_blogs_8/b/ii/posts/eda-in-the-1980s-the-dazzling-decadeof-electronic-design-automation.
11. Tao, F., Zhang, M. Digital twin shop-floor: a new shop-floor paradigm towards smart manufacturing. *IEEE Access. IEEE*, **2017**, *5*, 20418–20427.
12. Manyika, J., et al. *Big data: the next frontier for innovation, competition, and productivity* [Online]. McKinsey & Company Home Page, 2011 [Cited: 1 Dec 2014]. http://www.mckinsey.com/insights/business_technology/big_data_the_next_frontier_for_innovaton.
13. Zhuang, C., Liu, J., Xiong, H. Digital twin-based smart production management and control framework for the complex product assembly shop-floor. *Int. J. Adv. Manuf. Technol.*, **2018**, *96*(1–4), 1149–1163.
14. Parrott, A., Warshaw, L. *Industry 4.0 and the digital twin. Manufacturing meets its match* [Online]. 2017. https://www2.deloitte.com/content/dam/Deloitte/cn/Documents/cip/deloittecn-cip-industry-4-0-digital-twin-technology-en-171215.pdf.
15. Beaverstocks, M., Greenwood, A., Lavery, E., Nordgen, W. AppliedSimulation. *Modelling and analysis using FlexSim*, 4th edn., FlexSim Software Products, Inc., 2014.
16. OPC Foundation. *Home page—OPC foundation*. [Online]. 2018 [Cited: 22 Aug. 2018]. https://opcfoundation.org/.
17. Phan, H.T., Nguyen, N.T., Hwang, D. Convolutional attention neural network over graph structures for improving the performance of aspect-level sentiment analysis. *Inf. Sci.*, **2022**, *589*, 416–439.
18. Shekhawat, S.S., Shringi, S., Sharma, H., et al. Twitter sentiment analysis using hybrid Spider Monkey optimization method. *Evol. Intell.,* **2021**, *14*(3), 1307–1316.
19. Huddar, M.G., Sannakki, S.S., Rajpurohit, V.S., et al. Attention-based multi-modal sentiment analysis and emotion detection in conversation using RNN. *Int. J. Interact. Multimed. Artif. Intell.,* **2021**, *6*(6).
20. PengGuo. Quantum-inspired hierarchical attention mechanism for question answering. In *2021 IEEE 33rd International Conference on Tools with Artificial Intelligence (ICTAI),* IEEE, 2021, pp. 943–950.
21. Mittal, H., Saraswat, M., Bansal, J.C., Nagar, A. Fake-face image classification using improved quantum-inspired evolutionary-based feature selection method. In *2020 IEEE Symposium Series on Computational Intelligence (SSCI),* IEEE, 2020, pp. 989–995.
22. Chakraborty, S., Shaikh, S.H., Chakrabarti, A., Ghosh, R., et al. A hybrid quantum feature selection algorithm using a quantum inspired graph theoretic approach. *Appl. Intell.,* **2020**, *50*(6), 1775–1793.
23. Zhuang, C., Liu, J., Xiong, H. Digital twin-based smart production management and control framework for the complex product assembly shop-floor. *Int. J. Adv. Manuf. Technol.*, **2018**, *96*(1–4), 1149–1163.
24. Parrott, A., Warshaw, L. Industry 4.0 and the digital twin. Manufacturing meets its match [Online]. 2017. https://www2.deloitte.com/content/dam/Deloitte/cn/Documents/cip/deloittecn-cip-industry-4-0-digital-twin-technology-en-171215.pdf.

25. Beaverstocks, M., Greenwood, A., Lavery, E., Nordgen, W. AppliedSimulation. *Modelling and analysis using FlexSim*. 4th edn., FlexSim Software Products, Inc., 2014.
26. OPC Foundation. Home Page—OPC Foundation [Online]. 2018 [Cited: 22 Aug. 2018]. https://opcfoundation.org/.
27. Wei, Y., Hu, T., Dong, L., Ma, S. Digital twin-driven manufacturing equipment development. *Robot. Comput. Integr. Manuf.*, **2023**, *83*, 102557.
28. Lebjioui, S., Kaba Traoré, M., Ducq, Y. Digital twin-driven design: a framework to enhance system interoperability in the era of industry 4.0. In *International Conference on Interoperability for Enterprise Systems and Applications*, Springer: Cham, 2023, pp. 125–133.
29. Dauksher, R.; Patterson, Z.; Majidi, C. Characterization and Analysis of a Flexural Shape Memory Alloy Actuator. Actuators 2021, 10, 202. https://doi.org/10.3390/act10080202

CHAPTER 8

DEEP LEARNING METHODS IN MATERIAL SCIENCE

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ABSTRACT

Deep Learning refers to a subset of Machine Learning that utilizes artificial neural networks with multiple layers to extract data representations. These networks can predict outcomes, categorize data, and create original content. Deep Learning has driven substantial progress in areas like computer vision, natural language processing, and speech recognition. However, it demands sizable data sets and computational power to train models optimally. Consequently, while Deep Learning offers valuable solutions to intricate issues, it introduces concerns about privacy, bias, and energy usage.

8.1 DEEP LEARNING

One category within Artificial Intelligence and Machine Learning techniques, referred to as "Deep Learning," essentially represents a re-exploration of Artificial Neural Networks that were initially theorized in the 1980s. Neural Networks were effective in eliciting in the past few times thanks to the accessibility of large datasets as well as big computing, fulfilling its potential just being generic capable of understanding as well as modeling a number of processes. Deep Learning, a specialized branch of Machine Learning, offers several advantages, one of which is its ability to extract more detailed features from datasets.

This capability is rooted in the fusion of scientific computing principles and neural network intelligence. Deep adaptive algorithms have begun to outperform traditional methods in various everyday applications, such as image and speech recognition, online searches, identity verification, message filtering, credit risk assessment, and more. It has been demonstrated that Deep Learning approaches offer fascinating unique innovations in a variety of disciplines. Across many research disciplines, including chemical, quantum mechanics, biological, as well as materials engineering, Deep Learning methods have subsequently outperformed conventional learning-algorithm techniques. Deep Learning applications are still in their early stages, and the discipline has not fully explored their potential, implications, and limitations. Deep Learning offers fresh methods to examining structural occurrences and it has compelled resources researchers to broaden the scope of existing arsenal. It has recently been demonstrated that Deep Learning approaches may be employed in conjunction with quantum theory techniques for the material development. Although it is common to think that big samples were required in order for Deep Learning applications, methods like domain adaptation, inter models plus project-based learning may frequently make Deep Learning practical even for some tiny samples.

Substances are typically formed through a combination of theoretical understanding, practical applications, and a sound knowledge of chemistry principles. In contrast, the vast array of surface compositions make it impractical to explore them all in a timely and efficient manner. Therefore, the use of quantitative and analytical methodologies is necessary to effectively study and analyze these diverse compositions. While simulations are typically more efficient and cost-effective than experimental trials, their application in specific sectors is often limited by time constraints and timelines.

In contrast to conventional computer science methods, Deep Learning techniques have the potential to greatly enhance performance. In some instances, they have demonstrated accuracy on par with quantum theory and computational approaches.

Furthermore, establishing a new field of materials engineering requires qualifications, experience, specialized knowledge cultivation, and effective judgment to conduct thorough research. It is fortunate that we are currently residing in a time where network time and information are increasingly more accessible. When compared to other areas of study, Deep Learning research is notably more readily available for newcomers due to the presence of well-established and well-documented resources.

In the current era of data science, numerous fields, including research and engineering, are inundating us with vast amounts of information at an unprecedented pace. Consequently, a new paradigm of research known as data-driven science has emerged, leveraging large datasets generated by previous research endeavors. To effectively analyze such data and accelerate the development of new materials and achieve the goals of initiatives like the Composites Sequencing Program, enhanced statistical analysis methods are essential.

8.2 DEEP LEARNING BENEFITS AND DRAWBACKS

Deep Learning diverges from traditional machine learning methods in a few crucial aspects. As a result, it is essential to grasp these distinctions in order to ascertain the suitability of Deep Learning for a particular task. These characteristics, including both advantages and challenges, are depicted in Figure 8.1 and further elaborated below. When compared to traditional machine learning approaches, Deep Learning offers significant advantages.

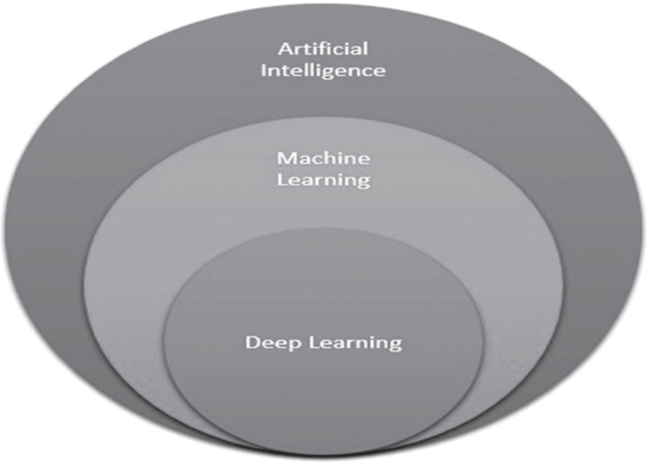

FIGURE 8.1 Showing relation between AI, ML, and Deep Learning.

1. The majority of Deep Learning is feature-free: The primary advantage of Deep Learning lies in its ability to effectively recognize trends within structured information, thereby significantly enhancing the

effectiveness of Machine Learning models. A good example often involves detailed manual features for a technological application, requiring expertise and substantial effort to design the necessary attributes. In contrast, Deep Learning can automatically identify key components in a dataset in a systematic manner, reducing the amount of work needed for classification techniques.

2. Big data generally improves the accuracy of Deep Learning: Each information Machine Learning model is anticipated to improve in correctness with further learning algorithm, although performance may saturation after a specific amount of time where after more supervised learning doesn't quite result in appreciable reliability improvements. Need plenty units are typically higher correct whenever vast information is recorded, despite the fact that classical Machine Learning- based algorithms seem to be accurate for smaller datasets and saturation considerably faster. This happens as a result of Deep Learning having more convolutions, which have a better generalization ability.
3. Deep Learning may generate recommendations more quickly: Despite being prohibitively costly, retraining algorithms only has a yet another expense. When developed correctly, robots were capable of foreseeing events quite quickly. Deep Learning seems to have the aforementioned benefits over conventional Machine Learning techniques, as well as several traits that can make several applications of that anyway difficult (Figure 8.2).

Deep Learning applications face four main difficulties:

1. Deep Learning needs a lot of data: The insufficient sequence information is occasionally the main barrier to deploying Deep Learning. Large information is typically necessary for Deep Learning, as it was stated previously. Large, carefully selected, well-labeled databases were uncommon across many academic and technical domains, including such structural engineering [2], notwithstanding the fact that these existed for more than just a number of issues including picture identification [1].
2. Big computation is required for Deep Learning: Despite the advancements in computer technologies, the task of continuously learning algorithms remains computationally taxing and time-consuming when dealing with large datasets. Another intriguing area of research lies in the potential for classical Deep Learning techniques to be harnessed [3, 4].

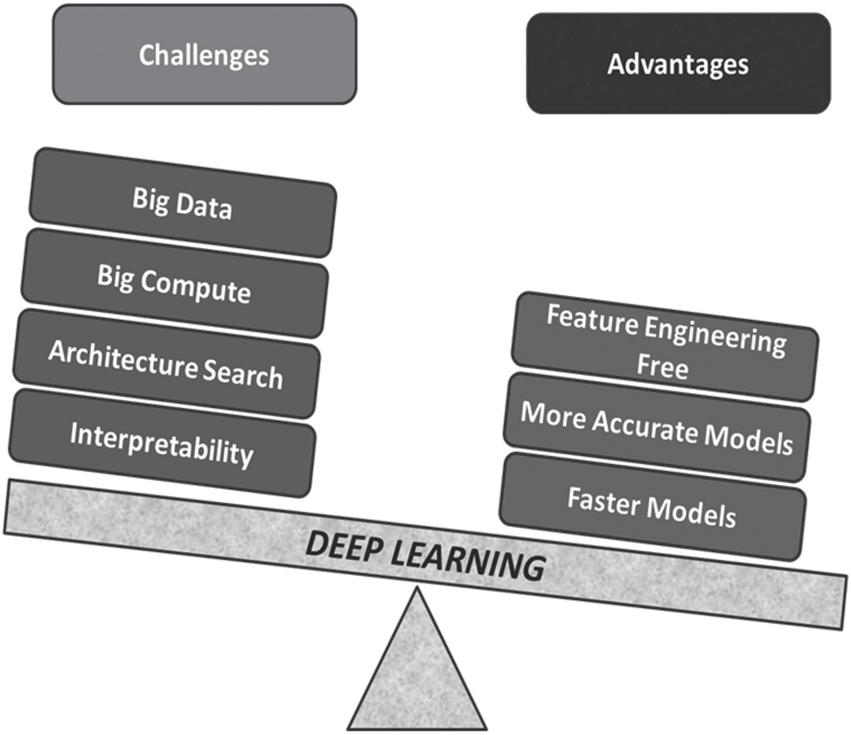
Challenges
Advantages
Big Data
Big Compute
Architecture Search
Interpretability
Feature Engineering Free
More Accurate Models
Faster Models
DEEP LEARNING

FIGURE 8.2 Showing advantage and challenges of Deep Learning. ⏎

3. Search for Deep Learning network infrastructure: These are countless efficient routing layouts because a convolutional layer is basically a collection of interlinked neurotransmitters. Determining the optimal architecture for a specific task, such as an assigned activity, lacks standardized systematic methods and remains an unresolved research area. Although there are fundamental guidelines based on past experiences that can help in selecting the appropriate architecture for a particular issue, further study is needed to fully address this complex topic [5].
4. Interpreting a Model: Because of their extreme complexity, Deep Learning-based techniques are commonly referred to that as “dark” algorithms. While attempts that methodically examine artificial neural functioning have already been made with certain amount of competence, in generally these cannot be as comprehensible as certain of the older predictive methods such predictor variables.

8.3 DEEP LEARNING: ESSENTIAL ELEMENTS AND IDEAS

The neuron serves as the fundamental computational unit within Artificial Neural Networks, incorporating various aspects of the system such as convolutions, including the geometric mean of these signals known as the convolution operation. A Deep Learning Network consists of an Artificial Neural Network with three or more convolutional nodes. The structure of this network is determined by the interconnections of synapses. Throughout Deep Learning, parameters were established for the vertices as well as connectivity among synapses again with aim of producing an outcome from an Artificial Neural Networks that is as truthful as feasible, a process known as minimizing the gradient descent. In order to increase overall durability of Deep Learning, signals were typically standardized to own declined in recent years plus equal sample variance [6]. The concept of regularization, simply known as regularization, allows for members to potentially apply regularization to convolution signals as well. The idea of breakdowns, where specific synapses are randomly deactivated during a forward or backward pass, is both helpful and intriguing within Artificial Neural Networks. This not only provides highly accurate approximations of inter average, but also acts as a regularization technique to reduce prediction error [7].

8.3.1 NEURAL NETWORKS WITH CONVOLUTIONS

Convolutional neural networks are a specific sort of Deep Learning algorithm with a variety of hyperparameters that are intended to have utilized on mapping, which include photographs. Utilizing CNN architecture, it is intended to accurately estimate geographically linked elements from pictures. Numerous components or filtering containing implementing possible or properties make up a fully connected layer. In order to generate complex patterns throughout the shape of wavelet coefficients, every screen is performed on the incoming picture as little more than a conducting different frame. These representations are utilized as parameters again for subsequent stage. In the initial stages of training a neural network, it is common to use pooled structures to reduce the dimensionality of the feature space. This process involves clustering algorithms to consolidate samples and coordinates, thereby decreasing the number of components and minimizing prediction errors [8, 9] (Figure 8.3).

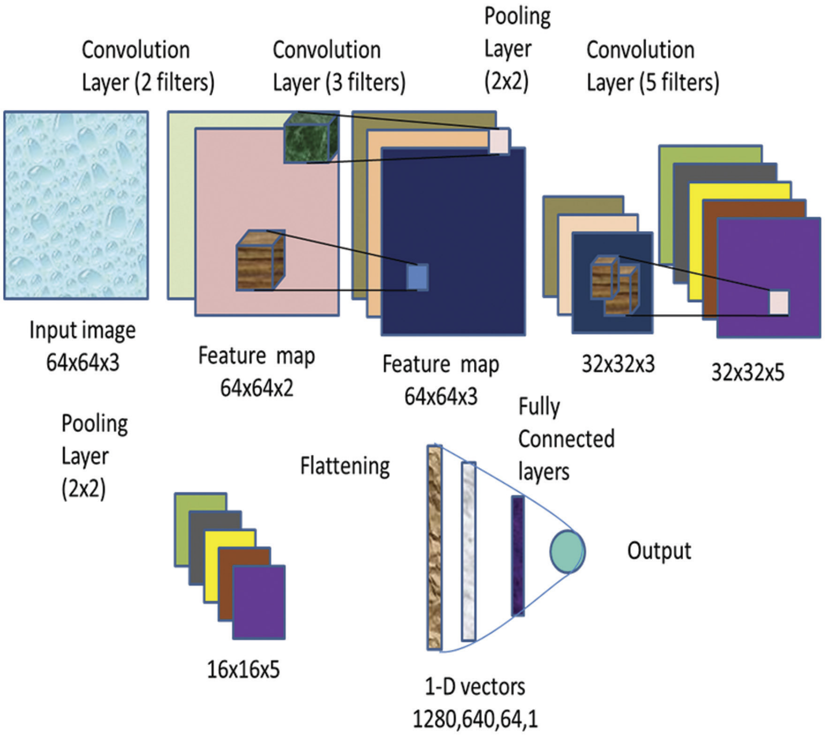
Convolution Layer (2 filters)
Convolution Layer (3 filters)
Pooling Layer (2x2)
Convolution Layer (5 filters)
Input image 64x64x3
Feature map 64x64x2
Feature map 64x64x3
32x32x3
32x32x5
Fully Connected layers
Pooling Layer (2x2)
Flattening
Output
16x16x5
1-D vectors 1280,640,64,1

FIGURE 8.3 A CNN having pooling layers, three fully linked layers, and three convolution layers. ⏎

8.3.2 *NEURAL NETWORKS*

1. Perceptron: The fundamental unit of Artificial Neural Networks seems to be the convolution, the artificial neurons [10], which conducts forwards propagating of signals. Most popular technology suites that support Neural Network training include PyTorch [11], Tensorflow [12], and MXNet [13]. Kindly be aware that, to accurately describe the technique, specific industrial apparatus and substances were also specified throughout this study. This designation neither supposed to suggest sponsorship as well as suggestion from NIST, nor is it meant to highlight that somehow the products indicated always represent the main contenders again for job.
2. Stimulation Function: The essential negative elements which allow neural nets to construct various small foundations to acquire

complicated effects include prominent ones, including convolution, batch normalization and Twirl. Like an illustration, the sigmoid activation function, which transfers actual figures toward the interval (0, 1), is frequently employed the final level of classification algorithm for represent probability. Both ultimate precision and supervisor support can be impacted by the convolution operation selected.

3. Normalization and Gradient Descent: The neurological cable network value matrix can either start off spontaneously or with data from something like a training sample. Updating models are produced by multiplying those edge weights even by input sequence as well as applying a nonlinear transformation. Such informed models are frequently convolution layers. Usually, conjugate gradient methods are implemented to continuously modify overall model parameters again till target precision is reached. In order to get another approximate solution of something like the damage equation in terms to each networking component via cyclical implementation of something like the following equation, the majority of contemporary Deep Learning algorithms use backward automated differentiating [14].
4. Regularization, underfitting, overfitting, and early stopping: The learning, validating, as well as testing set are separated from the information throughout a Machine Learning. Throughout learning, this testing set has never been employed. A simulation is considered to be something like if it underperforms upon that dataset but is unable to start learning the learning algorithm. When a product works satisfactorily on dataset examples yet poorly upon that validating, it is classified as majority of the cases [15]. Normalization strategies including dropouts, early halting, and L2 regularization can commonly be installed.
4. Networks of Generative Adversaries: The generative network, which derives form behavioral economics, represents one of the important intriguing types of Deep Learning Network designs in recent years. It is made up of not only one yet several algorithms which are competitively developed at the same time. A generative model, which became simply an inverted carrying out this project and up-samples an additive noise quaternion to a false persona, is among the structures. The differentiator utilizes a downsized representation of the source images to develop a probabilistic model, enabling classification as authentic or counterfeit. Figure 8.4 demonstrates Generative Adversarial Network principle. An analogy often used

to describe the process of a generator in a Generative Adversarial Network is likened to a burglar endeavoring to produce counterfeit currency, with the classification algorithm acting as the authorities tasked with distinguishing between genuine and fake money. This metaphor sheds light on the dynamic relationship at play within the network. When network nodes were training simultaneously, their gradually strengthen against one another until eventually reach the Balance point. [16] The discovery of intriguing implications in picture analytics by Generative Adversarial Networks, as highlighted in [17], should not come as a surprise. These implications include image quality computer vision, image restoration, retouching, as well as domains such as music composition.

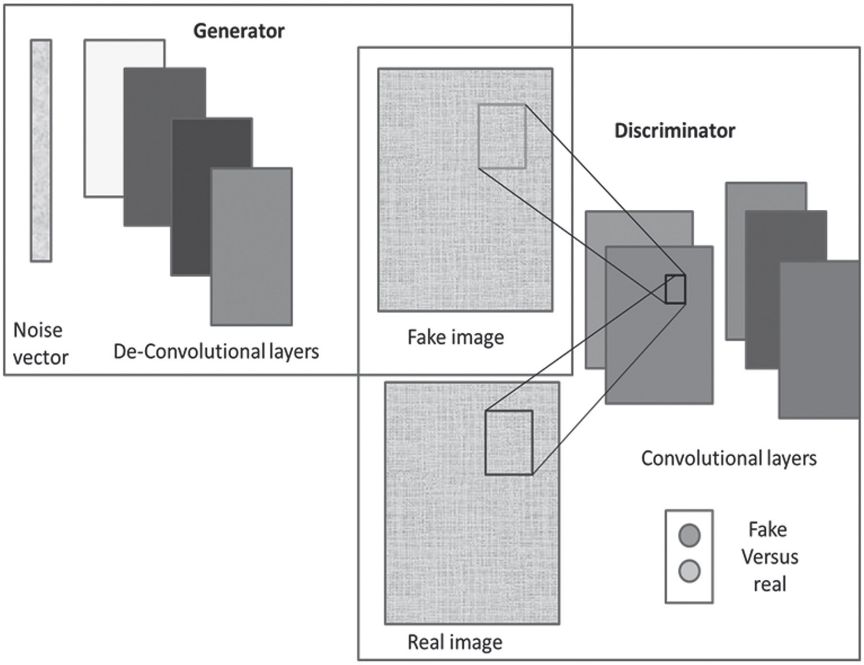
Generator
Noise vector
De-Convolutional layers
Fake image
Discriminator
Real image
Convolutional layers
Fake Versus real

FIGURE 8.4 Generative Adversarial Network consists of two neural networks—generator. ⏎

8.3.3 DEEP REINFORCEMENT LEARNING

Active Learning Algorithm is concerned with issues that occur when a computerized operator knows to choose a course of action through making mistakes. Deep Reinforcement Learning integrates Deep Learning into the Reinforcement Learning architecture to enable machines to depend solely learning information through metadata [18]. In conventional Reinforcement Learning, Decision optimizer is used, where an individual makes decisions for each linear interpolation to obtain a numerical payoff as well as transitioning to the subsequent subject to compliance with simulation model to establish strategy as well as increase profitability. Deep Learning approaches use strong variables as inputs, including continuous pictures.

8.3.4 ADDITIONAL DEEP LEARNING NEURAL NETWORK

There must be various additional Deep Learning Neural Network types that can analyze various sources of evidence in beyond the ones they have once again examined in this study (including Multilayer Perceptions, Convolutional Neural Network, as well as Generative Adviser able Networks).

The Recurrent Neural Network has the capability to operate with samples of various sizes, also known as sequential or time-series data. Its prominent applications lie in voice signals [19], Language Processing [20], and the potential advancements in materials computing [21, 22].

Geometrical Deep Learning is almost strange type of Deep Learning that can handle higher dimensional data, including networks containing different nodes, wherein convolutional Deep Learning modules are not clearly explained.

8.3.5 TRANSFER LEARNING

As previously noted, Deep Learning often requires large amounts of data. While the proposed method could help address challenges in Deep Learning when data is limited. Transfer learning works by sharing understanding from something like a Deep Learning approach built on huge information for one issue to another that is connected and then applying that understanding to develop a brand-new approach on increases and decreases for something like particular challenge. Since many substances databases are often limited in length in comparison to the massive statistics provided in various other fields, including Facebook, computational biology, astrophysics, and so on, Transfer Learning is anticipated to be particularly helpful for elements intelligence.

Object recognition commonly involves the use of machine learning algorithms such as VGG16 to analyze small image datasets and identify key features, ultimately creating efficient models [24]. ImageNet [25] is a collection of large libraries with further approximately 14 million thematic layers.

8.3.6 RESEARCH-BASED DEEP LEARNING

Many Deep Learning methods, including machine learning in particular, are showing promise for the future due to advancements in the emerging field of Scientific Deep Learning [26]. Another goal of Scientific Deep Leaning is to develop machine learning systems that bring together science expertise and physical class, whether immediately inside the designer's unique structure or implicitly throughout the retraining process' methodologies. In these kinds of systems, a Deep Learning model is often trained although several classical mechanics restrictions are applied [27–29]. The ability of a Neural Network to quickly learn irrelevant aspects of information, unrelated to variables a scientist would consider, poses a significant challenge for universal time series prediction. Employing particle normalization could help address this issue.

8.4 DEEP MATERIALS WITH EXAMPLES IN INFORMATICS

Next, we will examine several emerging uses of Deep Learning within material engineering to comprehend interactions using the other forward again and reverse modeling. Those instances further highlight the distinctive qualities of Deep Learning in the view of the elements that were normally mentioned.

One of the key advantages of Deep Learning is its ability to function effectively without the need for explicitly defined characteristics or subject matter expertise. This approach allows for immediate processing of input variables, making it a highly practical and efficient method, as mentioned earlier. In such an effort to feed the modeling existing chemical information, earlier research works [30–32] on production entropy predictions focused on the incorporation of thousands of type and concentration variables called physiological characteristics. Nevertheless, a phase like extracting features significantly relies on individual judgment and subject–matter knowledge. Additionally, it is often not feasible to finish the first stage for any and all situations because it might be challenging to convert the required subject -matter expertise into measured values for Machine Learning Algorithms of using.

8.4.1 INTERPRETABILITY OF MODELS

By several implementations, including corporate finance, driver assistance, as well as fabrication techniques, at which expense of a misdiagnosis could be immensely high, this same problem of prototype understandability always been essential. It is consequently essential to certify structure is not only quantifiable precise as well as acquiring knowledge again from desired specification as well as items that contribute to feeling, even though not understanding one that is recognized toward being untrue. In one of the initial attempts toward a comprehensive categorization of criteria and techniques based on probabilistic studies, Lipton [33] identified accessibility to individuals and interpretations of articles as integral factors, despite conflicting views on readability.

Understanding how a system operates from the perspective of a proposed approach involves grasping the significance of specific input variables and constants, as well as comprehending the overall functioning of a classification network. These aspects contribute to the transparent aspect of comprehensibility.

8.4.2 PROPERTY PREDICTION USING CRYSTAL STRUCTURE AWARENESS

Although structure approaches possessing the ability to be extremely precise, as illustrated in the case of the former, allotropes as well as constituents may display various characteristics for the same component. Forecasting material characteristics requires creating algorithms that take into account the architecture. Many researches [34, 35] use different types of features to convey the dataset for the Machine Learning algorithms to create forecasts. As shall be discussed more later, classifiers had been applied straight toward the crystalline lattice. Xie and Grossman [36] developed the Convolutional Neural Network framework for analyzing microstructures in crystalline materials. The method involves representing the crystalline nature as a graph, with endpoints indicating subatomic particles and corners representing connections between them. A Convolutional Neural Network incorporating various neural network techniques is then employed to optimize the modeling of desired characteristics. They used a library of 46,744 components [37] that included 216 spatial groupings, 7 framework structures, and 87 various pieces.

8.4.2.1 CRYSTAL STRUCTURE PREDICTION

Similar to molecular comprehensive solution in genomics, atomic level forecasting is still one of the major issues of components science [38, 39]. It is really possible to break the challenge of crystalline materials forecasting for more than just a mechanical mixture under mainly two fragments: initial production of alternative configurations as well as the following assessment of these same buildings to determine who is more probable (Figure 8.5).

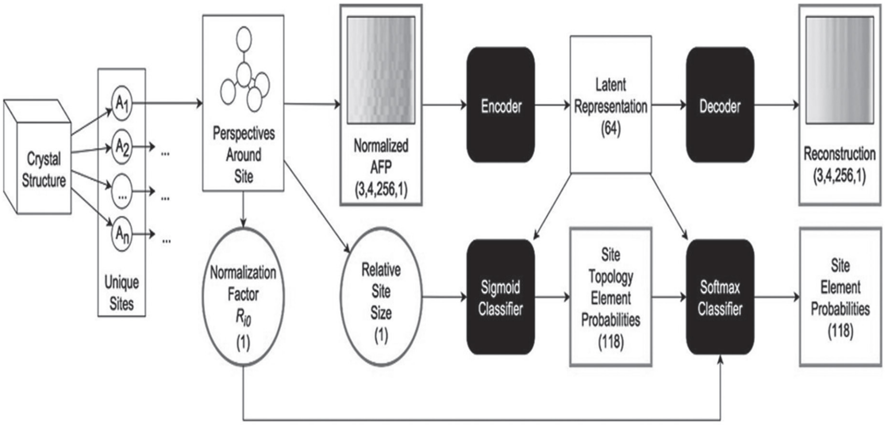
Crystal Structure
A_1
A_2
...
A_n
...
...
...
Unique Sites
Perspectives Around Site
Normalized AFP (3,4,256,1)
Encoder
Latent Representation (64)
Decoder
Reconstruction (3,4,256,1)
Normalization Factor R_{i0} (1)
Relative Site Size (1)
Sigmoid Classifier
Site Topology Element Probabilities (118)
Softmax Classifier
Site Element Probabilities (118)

FIGURE 8.5 Showing crystal structure prediction. ⏎

In general, optimization techniques utilizing various initial conditions [40] are commonly used in pattern-creation methods, with their effectiveness evaluated using quantum physics techniques. The likelihood of a crystal structure existing is estimated through a combination of probabilities for each component to occupy specific molecular positions after adjusting lattice parameters for forecasting purposes. Researchers transformed the initial challenge of estimating crystalline structures into predicting the probabilities of atomic or molecular positions within the structure, approximating the probability of a crystalline material's existence as the sum of probabilities for each component to occupy a specific atomic location.

Numerous viewpoints of normalized isotope fingerprinting were used as the appropriate signal of orbitals for the feature learning in order to record the surrounding topography surrounding every distinct radioactive site. This system was capable of comprehending architectural morphologies instead of crystalline structure having precise scales thanks toward the incoming representation's helpful properties like rotational parallelism, uniform dimensions, as well as preservation of three-dimensional knowledge. Several necessarily ensure made up the Deep Neural Network altogether.

Initially, the algorithm developed its own encoding for density functional fingerprinting by utilizing a 42-layer neural finite difference learning algorithm. This process effectively condensed the 3072-dimensional density functional fingerprinting into concise hidden interpretations to achieve its objective.

Now in order to determine whether mixtures of components were much more most likely to generate structure morphologies, those hidden characterizations were once again input everything into five logistic classifications. This same component particularly high risk was then formulated as a 118-class clustering algorithm by feeding the production likeliness form of the nonlinear activation discriminator into a five assistant autoencoder to regularization as well as 118 output units to anticipate which particular characteristic communicated toward the insight. This proposed technique, approximately represents 20% of something like the total sample size for molecular fingerprinting, has a mean RMSE of 31%, which is remarkably good for just a 118-class challenge.

It is intriguing to observe that most of the errors found in the approach appear to have some level of scientific plausibility. Additionally, an *t*-SNE (*t*-distributed variational neighbor autoencoder; [41]) incorporation of something like the nonlinear activation classifiers strength training again for components disclosed clusters corresponding to someone in the chemical components. This same Deep Learning approach's ability to pick up common themes as well as contaminant commonalities which were not board is responsible for ensuring to it during instruction merely besides learning from finely ground contextual features, comparable to the ElemNet framework [42] picked up from finely ground instrumentation samples, seems to be truly really very amazing.

8.4.3 FORCE-FIELD CONSTRUCTION

The development of Force Fields using Deep Learning [43, 44] and exploration of interparticle interactions is a critical component of the initial deployment. These applications offer numerous advantages, such as the capacity to address the unstable progression of Force and rapidly derive conclusions. Nonetheless, a drawback is the requirement for a substantial amount of training data and highly complex methodologies. When creating neighboring atoms possibilities that transcend 0 K temperatures but also night before going to bed behavior using experiments, including those for nanomaterials [45], frameworks like the Behler–Parrinello Neural Net as well as its derivatives [46, 47] were included. Similar Force-Field models have been created for materials like silica and potassium along with liquid processes including fluids, methanol, and many organic materials [48] (Figure 8.6).

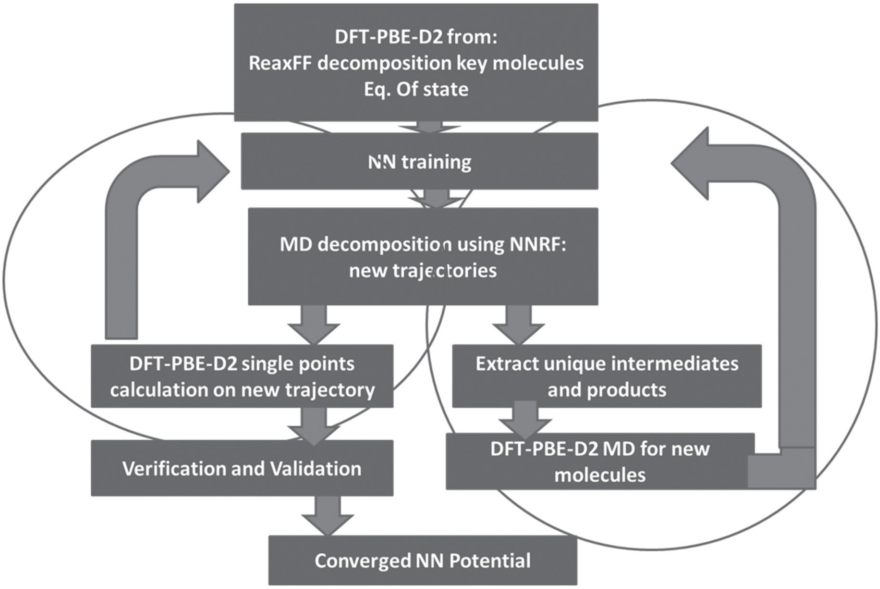
DFT-PBE-D2 from:
ReaxFF decomposition key molecules
Eq. Of state
NN training
MD decomposition using NNRF:
new trajectories
DFT-PBE-D2 single points
calculation on new trajectory
Extract unique intermediates
and products
Verification and Validation
DFT-PBE-D2 MD for new
molecules
Converged NN Potential

FIGURE 8.6 Showing force-field neural network structure. ⏎

While previous efforts primarily rely on Neural Networks, a new model known as the Graph Neural Network Force-Field [49, 50] has been created to overcome existing processing limitations. This innovative structure incorporates information extraction from the structural features that extend around the molecular positions and remain consistent, or rotate in the same direction as the measurement revolution. The accurate forecasting of molecular pressures can be achieved by this capability. Integrating regular force fields with neural networks, along with exploring potential relationships, could potentially help address issues in neural network calculations [51]. This approach may also contribute to the development of neural networks solely based on force fields.

8.4.4 INCREASED COMPOSITE WITH MULTIRESOLUTION HOMOGENIZATION AND LOCALIZATION LINKS

Throughout contrast to the earlier illustrations that also applied Deep Convolutional Network to constituents as well as crystalline materials information, the above subcategory examines applications of Deep Learning to three-dimensional metallographic information from two-phase blends for comprehending framework interconnections, who are also frequently needed to comprehended all over various distances. Normalization in this type of intermodeling entails the transmission of nanotechnology data between fewer timescales to greater timescales, for example, the predictions of macroscopic objects' properties knowing their architecture data. Transferring important substructure data from a greater size range to a smaller size range is what localization is all about (Figure 8.7).

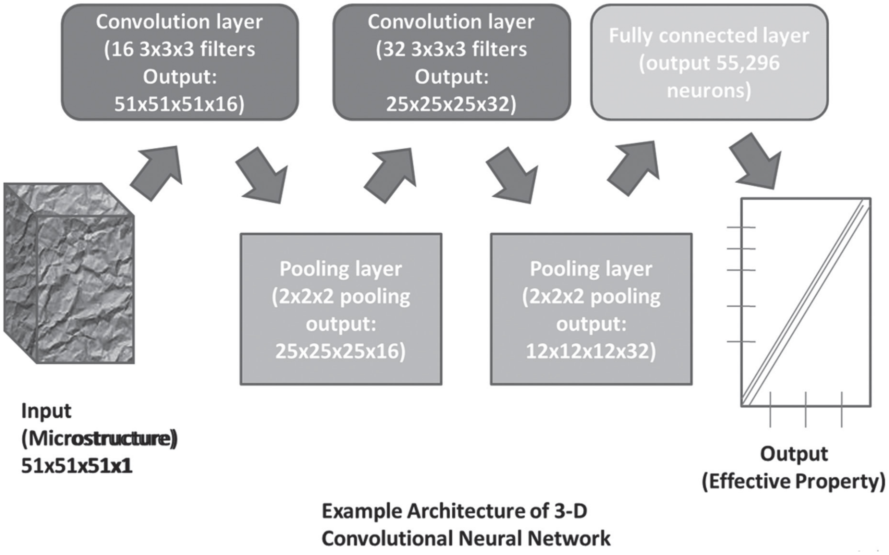
Convolution layer
(16 3x3x3 filters
Output:
51x51x51x16)
Convolution layer
(32 3x3x3 filters
Output:
25x25x25x32)
Fully connected layer
(output 55,296
neurons)
Pooling layer
(2x2x2 pooling
output:
25x25x25x16)
Pooling layer
(2x2x2 pooling
output:
12x12x12x32)
Input
(Microstructure)
51x51x51x1
Output
(Effective Property)
Example Architecture of 3-D
Convolutional Neural Network

FIGURE 8.7 Deep Learning approaches for mining structure property. ⏎

In the context of mechanics, localization refers to the distribution of stress at a microscopic scale within a specific component when exposed to a high load, such as pressure or elongation. Analytical calculations such as evolutionary algorithms utilizing Green's products or microscopic level finite difference computations used to explore simultaneous homogenized as well as relocation links simultaneously.

Materials knowledge systems [52] that also employ adjusted Green's mechanism granules in some kind of a noniterative numerical integration but instead Machine Learning-based algorithms that rely on data preprocessing to grab the neighborhood of something like the surface morphology, had already recently come to light as just a suitable strategy for recognizing language translation connections. A functionality learned in the classroom homogenized method for forecasting 0.3–0.6 presented excellent in two different hybrids of contrasting 50 is presented by Yang et al. [53]. The concept of contrast highlights differing characteristics of individuals' stage properties. In this specific case, it illustrates the relationship between the Young's moduli of the two periods. This collection included 8550 generated 3D nanostructures, also known as mesoscopic control volumes, with dimensions of 51 × 51 × 51. Remember that attribute is the consequence and architecture seems to be the reason again from interactions.

When compared with advanced quantum theory computer science techniques which use Principal Component Analysis two-point averages even though initial characteristics in extrapolation as well as simple quantum theory techniques or perhaps the principle of combinations methodology, the Deep Learning model's performance was demonstrated to be noticeably superior [54]. The study [55] discovered that the filtering and polynomial acquisition by the Network during development can be interpreted as nanoscale information crucial for attaining the desired cosmological scales attribute. This research utilized Deep Learning techniques to investigate the homogenized, additional study findings.

In a study conducted by Yang et al. [56], the sample set was partitioned into training, validation, and testing sets. The researchers employed distance measures such as Contrast-10 (2600) and Contrast-50 (3300) with a dimension of 21 × 21 × 21, incorporating varying current capacity and periodic finite elements.. Every vox serves as an information source for the estimation challenges, hence the focusing region was represented by a 3D neighborhood with dimensions of 11 × 11 × 11. Researchers achieved this through considering the 11 × 11 × 11 3D information as 11 bands of an 11 × 11 2D frame, transverse of maximal primary tension. With this issue, a Network model comprising seven layers convolutional and two specially layers—performed reasonably optimum. The technique [57], 2 Machine Learning-based approaches termed single approach [58] as well as inter approach [59], although this is simply a multilevel extension of the specific methodology, were used to evaluate the precision of the Deep-Learning network (Figure 8.8).

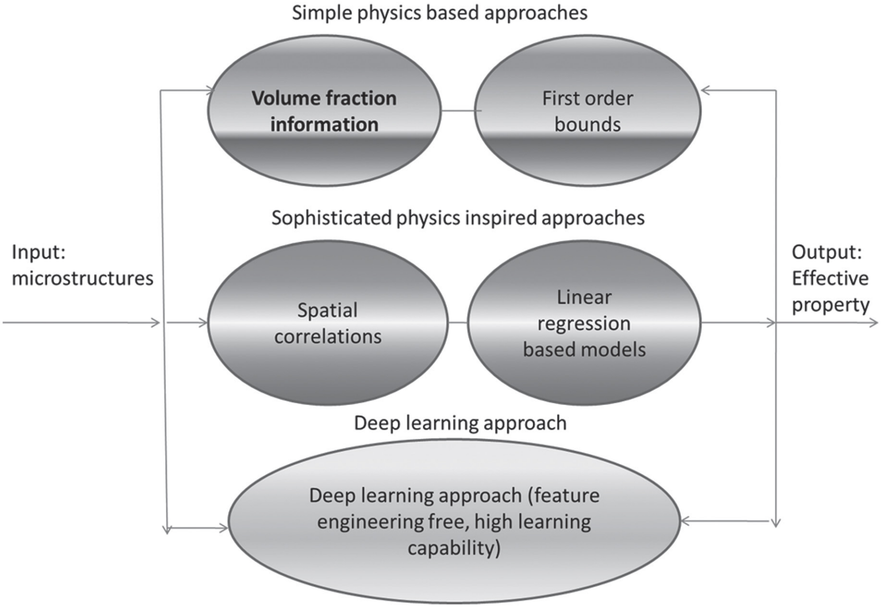
Simple physics based approaches
Volume fraction information
First order bounds
Sophisticated physics inspired approaches
Input: microstructures
Spatial correlations
Linear regression based models
Output: Effective property
Deep learning approach
Deep learning approach (feature engineering free, high learning capability)

FIGURE 8.8 Deep Learning approach for property linkage. ⏎

8.4.5 DESIGN AND RECONSTRUCTION OF THE MICROSTRUCTURE

Another major challenge in modeling heterogeneity substances is how to reconstitute the architecture of a disorderly heterogeneity substance utilizing scant architectural data from the initial system [60]. A Deep transferable Learning-based method was created by Li et al. [61] enabling rebuilding substantially comparable crystallites from any particular composite based on a personal morphology. In order to provide an intake to something like a reduced variant of a classifier Network dubbed VGG16, our method first encodes the incoming substructure with k identified methodology is based to a 3 approximation [62]. Additional training set Grayscale picture is also being transmitted to trimmed VGG16 network at the same time. This vision will eventually be modified to produce the encrypted substructure restoration.

This discrepancy among the installations of something like the existing as well as replicated architecture, added over a few neural networks of something like the trimmed VGG16, is the algorithm that needs to be reduced [63].

This divergence of something like the damage changes to the network parameters is commonly determined throughout artificial neural development in order to repeatedly optimize the weights and improve the models. However, in this case, the program's strengths were fixed, as well as the parameters up for optimization are indeed the input data of the nonlinear mapping reconstituted substructure. In order to repeatedly modify this same number of pixels of the substructure reconstructions until it corresponds, calculated gradients of something like the crushing defeat without reference toward every component inside the recreated architecture is determined using transfer learning and then supplied together into stochastic approach (Figure 8.9).

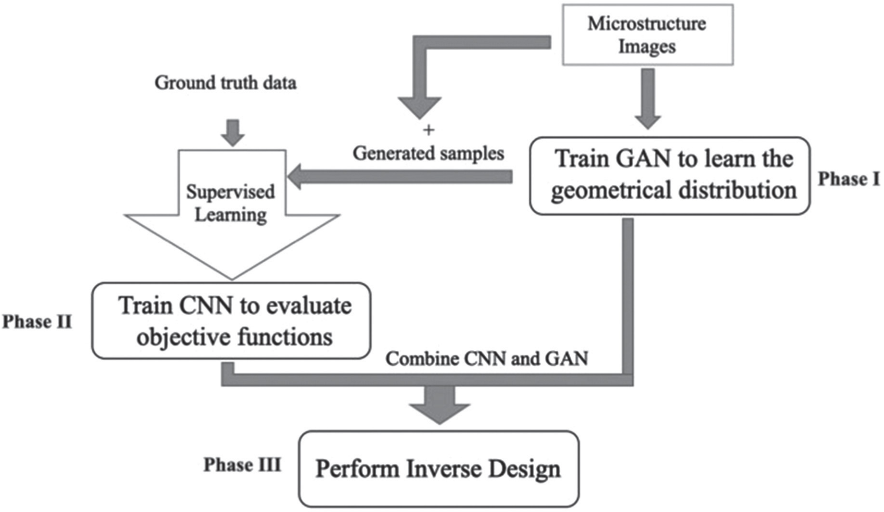
Microstructure Images
Ground truth data
+
Generated samples
Train GAN to learn the geometrical distribution
Phase I
Supervised Learning
Phase II
Train CNN to evaluate objective functions
Combine CNN and GAN
Phase III
Perform Inverse Design

FIGURE 8.9 Microstructural design using Deep Learning. ⏎

These volumetric percentages might not be exactly the same as the underlying substructure, which is undesirable. That phasing labeling of a portion of the border regions was nonetheless changed in a subsequent article stage employing evolutionary algorithms in order to better align the mixture percentages inside the underlying as well as rebuilt crystallites.

The same approach has been found to outperform specific strategies such as judgment decision trees synthesizing [64], Gaussian distribution sector [65], 2-point cointegration, and physiological signifier [66] in four out of five industrial applications. This was confirmed after a thorough evaluation across a wide range of engineering morphological features.

One of the key challenges in materials science and engineering is the development of substructures. Identifying suitable abstractions for substructure development is a crucial task in working toward this objective.

8.4.6 DEGRADATION DETECTION

Deep Learning is a more accurate and efficient method for analyzing materials to detect metal dissolution, pavement surface cracks, and fine aggregates compared to relying on subjective judgments [67, 68]. Agrawal et al. (1996) investigated the link between physicochemical characteristics of something like the aluminum yet its materials and industrial production operating parameters to investigate numerous functions inside which Deep Learning methods (including such image segmentation and forecasting) are employed to anticipate the exhaustion load bearing capacity.

This tempered temperature was shown to be the largest significant factor that influences endurance resistance out of the 25 characteristics that were examined. There are four stages of the procedure: First, the underlying information is typically normalized with technical knowledge. Second, sensitively characteristics were chosen using performance-rating techniques. The permanent deformation was then predicted using Deep Learning algorithms.

Finally, associated with inefficient was employed to assess the algorithms' accuracy. These findings demonstrate that numerous Deep Learning techniques, including regression analysis and Artificial Neural Network achieved great generalization ability, including Adjusted r^2 >.98 as well as margins of error 4%.

Zhang presented a CNN-based, perform effectively with input image precision. It had a high degree of precision of 90.13% when detecting sidewalk fractures using (3D) photographs of such a subgrade layer. Another adapts for railroad track inspections were suggested in a framework developed by Gibert et al. [94]. Depending on something like a deep network.

In the process of substance categorization, four classifiers were employed, followed by the use of five convolutions for fastening identification. A specially designed programming language was used to analyze the material, after investigators gathered 203 track photos covering a total of 84 km using a vehicle equipped with artificial lighting. Eighty percent of the photos were allocated for retraining purposes, while the remaining 20% were reserved for assessment within the five categories related to the collected data. Subsequently, 50,000 pieces were randomly selected for data fusion in each category, resulting in a total of 1.5 million squares being utilized to train each algorithm.

8.4.7 COMPONENT-FOCUSED DESIGN

Considering giving accurate makeup, Deep Learning has the ability to anticipate active chemicals as well as associated architectures [69]. A total of

209 novel quaternary compounds were found using a prediction algorithm predicated on an observational crystallographic dataset. Meredig et al. also developed a Learning forecasting algorithm for potential physicochemical characteristics of unpredictable combinations that would have been built on hundreds of simulation results. Several prediction construction energies frameworks as well as a sizable collection of computed values were created by the scientists. Researchers subsequently scanned 1.6 million prospective quaternary composition using those same different modalities, combined the rankings between the most likely outcomes, and discovered 4500 point of equilibrium substances [70].

In a study with a similar focus, Deep Learning was used to analyze multimodal compounds. An initial group of 67 octahedral substances was divided into distinct categories based on their crystalline structures utilizing a transfer learning automated system. Subsequently, a Deep Learning model was employed to accurately determine the conformations of 55 compounds [71]. Eventually, a correlation methodology was employed to anticipate the transition temperature of molecules by excavating a mixture of sixteen qualities from each bitwise facility's atoms. Deep Learning had also proven to be highly accurate in the experiments mentioned previously as well as the ability to find substances.

Additionally, a method has been introduced for producing unique metabolites with specific biochemical characteristics and physical properties through a compensation process. This method is based on observation algorithms and consists of two essential components: a generator/ing and a classifier [72]. The generating collects the characteristics of samples, as well as the differentiator determines whether another emitter monomer may occur by comparing it to actual microstructures. This generating is conditioned to increase the individual false alarm rate. Continuing this procedure will improve the individual ability to distinguish among authentic and fraudulent information. Consequently, a reinforcement learning networks that includes a "compensation function" could be utilized to develop molecules with unique genetic properties. The structure of this overarching goal feedforward neural network is illustrated in Figure 8.10.

8.4.8 SPECTRAL MODELS

A spectrophotometer indication is created whenever visible light interacts with a substance and is determined as a result of the radiation's spectral distribution. Approach is to examine more about the content, structure, and harmonic components of substances by researching spectrophotometer. Spectrometric methods are essential for characterization of substances. For almost a decade, cross scattering has been used to determine the crystalline phase of many substances. Adapting qualitative numerical simulations can be done by spectral methods, since many experimental methods include adapting cubic permutations of spectral could be done through cross absorbance located close spectrometry (Figure 8.11).

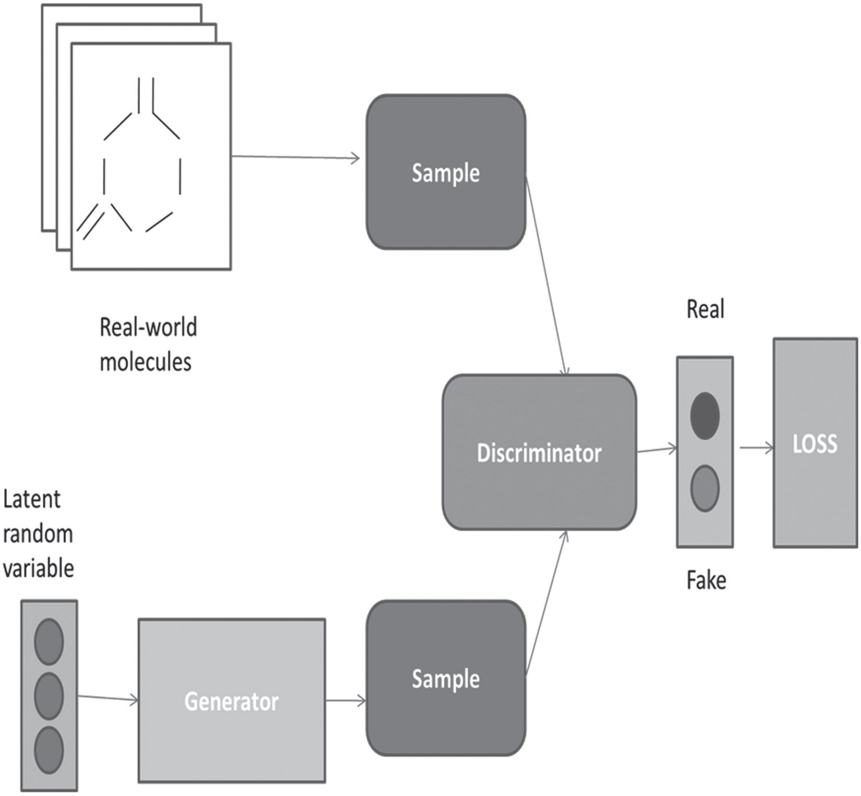

FIGURE 8.10 Framework of an objective-reinforced generative adversarial network. ⏎

A meticulous planning of investigations, the description, modification, and continuous matching of mathematical model, or the accessibility of reference wavelengths of well-known substances all call for a greater extent of investigator experience including both strategies. Spectrographic information has increased recently as a result of improvements in elevated operations and computerized information, providing chances for academics to understand from inside the information but perhaps displacing traditional approaches in their analysis. In order to provide real instances as well as perspectives, this report explains new Deep Learning implementations in several methods of spectroscopy information processing.

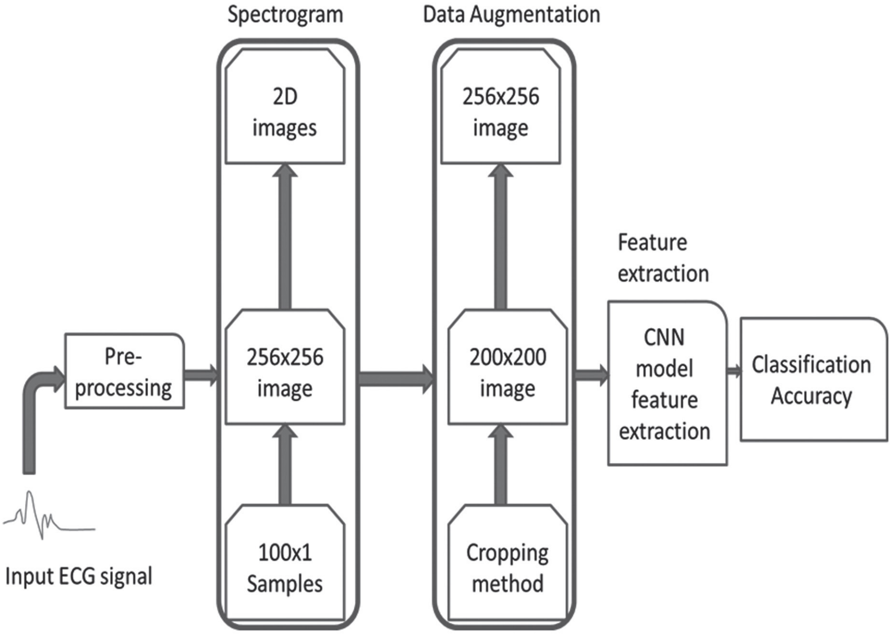
Spectrogram
Data Augmentation
2D images
256x256 image
Feature extraction
Pre-processing
256x256 image
200x200 image
CNN model feature extraction
Classification Accuracy
Input ECG signal
100x1 Samples
Cropping method

FIGURE 8.11 Spectral image using Deep Learning. ⏎

8.4.9 MESOSCALE MODELING USING DEEP LEARNING

Deep Learning techniques are being applied in macroscopic level modeling more and more in complement to appearance evaluation. By including an average confidence interval of 10%, Dai et al. [73] effectively trained a Graphical Neural Network to anticipate studies that have found a link in a variety of artificial heterogeneous environments. A network is used to depict the substructure, with each node standing for a heaping teaspoon as well as the connections connecting nodes denoting the boundaries among adjacent granules.

After considering the relationships between neighboring particles, the Graphical Neural Network outperformed earlier Deep Learning approaches in forecasting properties of diverse substances (Figure 8.12).

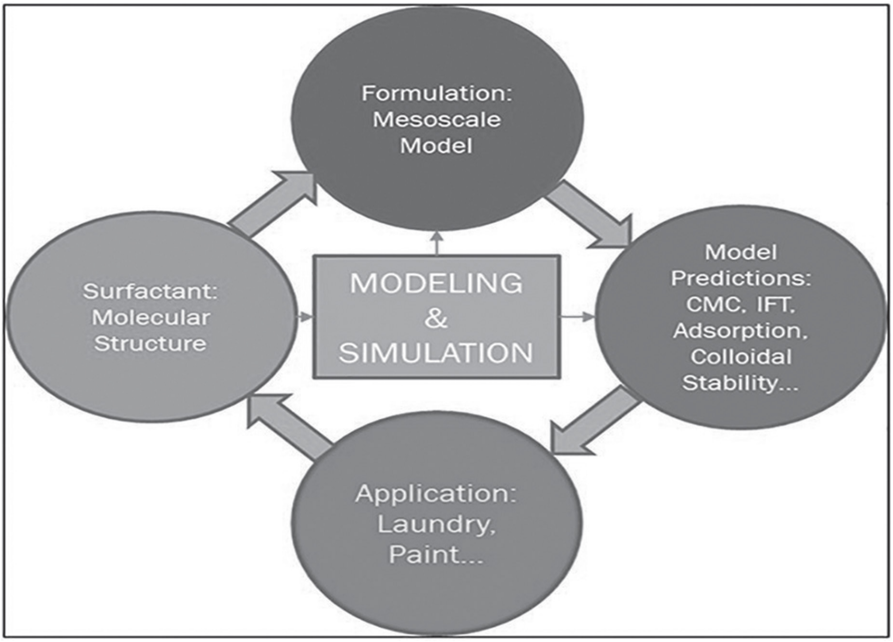
Formulation:
Mesoscale
Model
Model
Predictions:
CMC, IFT,
Adsorption,
Colloidal
Stability...
Application:
Laundry,
Paint...
Surfactant:
Molecular
Structure
MODELING
&
SIMULATION

FIGURE 8.12 Diagram showing mesoscale modeling. ⏎

Comparable initial research using Graphical Neural Network to forecast the incidence of aberrant grain growth in Monte Carlo analyses of surface texture is presented by Cohn and Holm253. Under certain substances, aberrant grain growth is famously challenging to anticipate, manage, and moreover empirically detect since it seems to be random. Although aberrant grain growth has been replicated in Monte Carlo simulations of industrial applications, there is currently no framework which might anticipate whether beginning micrographs will pass through aberrant grain growth. Utilizing SPPARKS254255, a collection of Monte Carlo simulations was produced. With something like a recognition rate of 75%, a substructure Graphical Neural Network was trained to predict particular experiments. The efficiency of a graphics system was just 60%. Its Graphical Neural Network also offered tangible explanations and showed which only three neighborhood casings are required to reach the report's high productivity. The above preliminary findings encourage further investigation into the use of Graphical Neural Network to forecast incidence across both modeled as well as actual substances throughout production.

8.5 LIMITATIONS AND CHALLENGES

Although Deep Learning approaches present numerous opportunities for both preparation and application, they also come with certain limitations and areas for enhancement. It can be challenging to ascertain the reliability and accuracy of data utilized in Deep Learning tasks due to inadequate regression coefficients, insufficient indicators for inclusion in the United States, or potentially irreproducible information using similar predetermined criteria [74]. This presents a significant obstacle to Deep Learning-based forecasting. Materialist depictions based on molecular formulas typically do not consider organization, making them less adaptable to working with natural drugs where architectural knowledge may be lacking. This limitation also hinders their ability to accurately capture events such as phase transformations. The characteristics of substances can vary significantly depending on their nanostructure, as seen in the contrast between sapphire and graphene. It is not uncommon for the procedures used for formulas to be ineffective in these cases.

Atomic diagram projections are often mistakenly perceived as a complete essentialist characterization. In reality, their evaluation is primarily based on bulk counterparts rather than on imperfect subsystems or on the number of space travel stages. This is especially noticeable when taking a hybrid approach. This emphasizes that the model parameters would have to be accurate predictors of the outcome categories and that they should not omit any essential data.

These observational results are frequently extremely complex in dimensions of pictures and spectroscopy, necessitating extensive processing before using Deep Learning. While supposition-predicted values offer an alternative course of action, they cannot accurately reflect real-world situations like the existence of unstructured interference [75].

Additionally, we emphasize the challenging scientific endeavor of establishing a closed-loop autonomous equipment development and manufacturing system [76, 77] capable of integrating experimentation and Deep Learning modules concurrently within a controlled environment.

The gaseous component for something like a following trial was again dynamically changed depending on the preceding investigations, without involving a supervisor, to independently approach forward into a desired metal redox potential [78]. Only a small portion of everything that is ultimately conceivable is shown by this straightforward demonstration of the concept exercise.

8.6 POSSIBLE LONG-TERM EFFECTS

The fundamental elements for human advancement are resources. The advancement of society relies on the development of superior, healthier, faster, cost-effective, and environmentally sustainable products. Deep substance information systems have the potential to revolutionize the field of substance engineering and science by understanding how individuals efficiently narrow down a vast array of candidates to a select few for testing with computer models. This process leads to reduced costs and accelerated development of state-of-the-art components. In order to accomplish the Machine vision, Deep commodities bioinformatics holds out exceptional possibilities for accelerating both identification as well as creation toward the next involves a combination that is both efficient as well as expensive. The utilization of deep substance analytics may potentially impact various industries in real life, such as aeronautical, automotive, clean technology, architecture, wellness, and mobility.

KEYWORDS

- **deep Learning**
- **advantage**
- **disadvantage**
- **application**

REFERENCES

1. Deng, J., Dong, W., Socher, R., Li, L.J., Li, K., Fei-Fei, L. ImageNet: a large-scale hierarchical image database. In *2009 IEEE Conference on Computer Vision and Pattern Recognition*, Miami, FL, June 20–25, 2009, pp 248–255. https://doi.org/10.1109/CVPR.2009.5206848.
2. Agrawal, A. Choudhary, A. Perspective: materials informatics and big data: realization of the “fourth paradigm” of science in materials science. *APL Mater.*, **2016**, *4*, 053208.
3. Lee, S., Jha, D., Agrawal, A., Choudhary, A., Liao, W.-K. Parallel deep convolutional neural network training by exploiting the overlapping of computation and communication. In *24th IEEE International Conference on High Performance Computing, Data, and Analytics (HIPC)*, 2017, pp. 183–192.

4. Mnih, V., Badia, A.P., Mirza, M., Graves, A., Lillicrap, T., Harley, T., Silver, D., Kavukcuoglu, K. Asynchronous methods for deep reinforcement learning. In *International Conference on Machine Learning*, 2016, pp. 1928–1937.
5. Patton, R.M., Johnston, J.T., Young, S.R., Schuman, C.D., March, D.D., Potok, T.E., Rose, D.C., Lim, S.H., Karnowski., T.P., Ziatdinov, M.A., Kalinin, S.V. 167-PFlops deep learning for electron microscopy: from learning physics to atomic manipulation. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis*, IEEE Press, 2018, p. 50.
6. Lou, Y., Caruana, R., Gehrke, J. Intelligible models for classification and regression. In *Proceedings of 18th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. ACM, 2012, pp. 150–158
7. Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., Salakhutdinov, R. Dropout: a simple way to prevent neural networks from overfitting. *J. Mach. Learn. Res.*, **2014**, *15*, 1929–1958.
8. Kipf, T.N., Welling, M. Semi-supervised classification with graph convolutional networks. 2016. arXiv: https://arxiv.org/1609.02907.
9. Zhou, J., Cui, G., Zhang, Z., Yang, C., Liu, Z., Sun, M. Graph neural networks: a review of methods and applications. 2018. arXiv https://arxiv.org/1812.08434.
10. Minsky, M., Papert, S. A. *Perceptrons: an introduction to computational geometry*. MIT Press, 2017.
11. Paszke, A., et al. Pytorch: an imperative style, high-performance deep learning library. *Adv. Neural Inf. Process. Syst.*, **2019**, *32*, 8026–8037.
12. Abadi, et al. TensorFlow: a system for large-scale machine learning. 2006. arXiv: https://arxiv.org/abs/1605.08695.
13. Chen, T., et al. Mxnet: a flexible and efficient machine learning library for heterogeneous distributed systems. 2015. arXiv: https://arxiv.org/abs/1512.01274..
14. Baydin, A.G., Pearlmutter, B.A., Radul, A.A., Siskind, J.M. Automatic differentiation in machine learning: a survey. *J. Machine Learn. Res.*, **2018**, *18*, 1–43.
15. Artrith, N., et al. Best practices in machine learning for chemistry. *Nat. Chem.*, **2021**, *13*, 505–508.
16. Osborne, M.J. Rubinstein, A. *A course in game theory*. MIT Press: Cambridge, MA, 1994, p. 14, ISBN 9780262150415.Google Scholar
17. Wang, T., Liu, M., Zhu, J., Tao, A., Kautz, J., Catanzaro, B. *High-resolution image synthesis and semantic manipulation with conditional GANs*. CVPR, 2018.
18. Pereira, T., Abbasi, M., Ribeiro, B., Arrais, J.P. Diversity oriented deep reinforcement learning for targeted molecule generation. *J. Cheminformatics*, **2021**, *13*, 1–17.
19. Miao, Y., Gowayyed, M., Metze, F. EESEN: end-to-end speech recognition using deep RNN models and WFST-based decoding. In *2015 IEEE Workshop on Automatic Speech Recognition and Understanding (ASRU)*, Scottsdale, AZ, December 13–17, 2015, pp. 167–174. https://doi.org/10.1109/ASRU.2015.7404790.Google Scholar
20. Xie, Y., Daga, P., Cheng, Y., Zhang, K., Agrawal, A., Choudhary, A. Reducing infrequent-token perplexity via variational corpora. In *53rd Annual Meeting of the Association of Computational Linguistics (ACL) and 7th International Joint Conference on Natural Language Processing*, 2015, pp. 609–615.
21. Mozaffar, M., Paul, A., Al-Bahrani, R., Wolff, S., Choudhary, A., Agrawal, A., Ehmann, K., Cao, J. Data-driven prediction of the high-dimensional thermal history in directed energy deposition processes via recurrent neural networks. *Manuf. Lett.*, **2018**, *18*, 35–39.

22. Paul, A., Jha, D., Al-Bahrani, R., Liao, W.-K., Choudhary, A., Agrawal, A. CheMixNet: mixed DNN architectures for predicting chemical properties using multiple molecular representations. *NIPS Workshop on Machine Learning for Molecules and Materials (MLMM)*. 2018, arXiv: https://arxiv.org/1811.08283..
23. Gatys, L., Ecker, A.S., Bethge, M. Texture synthesis using convolutional neural networks. In *Proceedings of Advances in Neural Information Processing Systems (NIPS)*, 2015, pp. 262–270.
24. Gopalakrishnan, K., Khaitan, S.K., Choudhary, A., Agrawal, A. Deep convolutional neural networks with transfer learning for computer vision-based data-driven pavement distress detection. *Constr. Build. Mater.*, **2017**, *157*, 322–330.
25. Deng, J., Dong, W., Socher, R., Li, L.J., Li, K., Fei-Fei, L. ImageNet: a large-scale hierarchical image database. In *2009 IEEE Conference on Computer Vision and Pattern Recognition*, Miami, FL, USA, June 20–25, 2009, pp. 248–255. https://doi.org/10.1109/CVPR.2009.5206848.\
26. Baker, N., et al. Workshop report on basic research needs for scientific machine learning: core technologies for artificial intelligence. *Tech. Rep.*, **2019**. https://doi.org/ 10.2172/1478744.
27. Chan, H., et al. Rapid 3d nanoscale coherent imaging via physics-aware deep learning. *Appl. Phys. Rev.*, **2021**, *8*, 021407.
28. Pun, G.P., Batra, R., Ramprasad, R., Mishin, Y. Physically informed artificial neural networks for atomistic modeling of materials. *Nat. Commun.*, **2019**, *10*, 1–10.
29. Onken, D., et al. A neural network approach for high-dimensional optimal control. 2021 arXiv. https://arxiv.org/abs/2104.03270.
30. Jha, D., Ward, L., Paul, A., Liao, W.-K., Choudhary, A., Wolverton, C., Agrawal, A. Elemnet: deep learning the chemistry of materials from only elemental composition. *Nat. Sci. Rep.*, **2018**, *8*, 17593.
31. Meredig, B., Agrawal, A., Kirklin, S., Saal, J.E., Doak, J.W., Thompson, A., Zhang, K., Choudhary, A., Wolverton, C. Combinatorial screening for new materials in unconstrained composition space with machine learning. *Phys. Rev. B*, **2014**, *89*, 1–7.
32. Ward, L., Agrawal, A., Choudhary, A., Wolverton, C. A general-purpose machine learning framework for predicting properties of inorganic materials. *npj Comput. Mater.*, **2016**, *2*, 16028..
33. Lipton, Z.C. The mythos of model interpretability. *Commun. ACM*, **2018**, *61*, 36–43. https://doi.org/10.1145/3233231
34. Schütt, K.T., Glawe, H., Brockherde, F., Sanna, A., Müller, K.R., Gross, E.K.U. How to represent crystal structures for machine learning: towards fast prediction of electronic properties. *Phys. Rev. B*, **2014**, *89*, 205118. https://doi.org/10.1103/PhysRevB.89.205118
35. Faber, F., Lindmaa, A., Anatole von Lilienfeld, O., Armiento, R. Crystal structure representations for machine learning models of formation energies. *Int. J. Quantum Chem.*, **2015**, *115*, 1094–1101.
36. Xie, T., Grossman, J.C. Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties. *Phys. Rev. Lett.*, **2018**, *120*, 145301. https://doi.org/10.1103/PhysRevLett.120.145301
37. Jain, A., Ong, S.P., Hautier, G., Chen, W., Richards, W.D., Dacek, S., Cholia, S., Gunter, D., Skinner, D., Ceder, G., Persson, K.A. Commentary: the materials project: a materials genome approach to accelerating materials innovation. *APL Mater.*, **2013**, *1*, 011002.
38. Oganov, A.R. (Ed.). *Modern methods of crystal structure prediction*. John Wiley & Sons: Hoboken, NJ, USA, 2011.

39. Dill, K.A., Ozcan, S.B., Weikl, T.R., Chodera, J.D., Voelz, V.A. The protein folding problem: when will it be solved? *Curr. Opin. Struct. Biol.*, **2007**, *17*, 342–346.
40. Gautier, R., Zhang, X., Hu, L., Yu, L., Lin, Y., Sunde, T.O., Chon, D., Poeppelmeier, K.R., Zunger, A. Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds. *Nat. Chem.*, **2015**, *7*, 308. https://doi.org/10.1038/nchem.2207
41. Van der Maaten, L., Hinton, G. Visualizing data using t-SNE. *J. Mach. Learn. Res.*, **2008**, *9*, 2579–2605.
42. Jha, D., Ward, L., Paul, A., Liao, W.-K., Choudhary, A., Wolverton, C., Agrawal, A. Elemnet: deep learning the chemistry of materials from only elemental composition. *Nat. Sci. Rep.*, **2018**, *8*, 17593.
43. Smith, J.S., Isayev, O., Roitberg, A.E. Ani-1: an extensible neural network potential with DFT accuracy at force field computational cost. *Chem. Sci.*, **2017**, *8*, 3192–3203.
44. Behler, J. Atom-centered symmetry functions for constructing high-dimensional neural network potentials. *J. Chem. Phys.*, **2011**, *134*, 074106.
45. Weinreich, J., Romer, A., Paleico, M.L., Behler, J. Properties of alpha-brass nanoparticles. 1. neural network potential energy surface. *J. Phys. Chem. C*, **2020**, *124*, 12682–12695.
46. Behler, J., Parrinello, M. Generalized neural-network representation of high-dimensional potential- energy surfaces. *Phys. Rev. Lett.*, **2007**, *98*, 146401.
47. Ko, T.W., Finkler, J.A., Goedecker, S., Behler, J. A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer. *Nat. Commun.*, **2021**, *12*, 398.
48. Wang, H., Zhang, L., Han, J., E, W. DeePMD-kit: a deep learning package for many-body potential energy representation and molecular dynamics. *Comput. Phys. Commun.*, **2018**, *228*, 178–184.
49. Park, C.W., et al. Accurate and scalable graph neural network force field and molecular dynamics with direct force architecture. *npj Comput. Mater.*, **2021**, *7*, 1–9.
50. Chmiela, S., Sauceda, H.E., Müller, K.-R., Tkatchenko, A. Towards exact molecular dynamics simulations with machine-learned force fields. *Nat. Commun.*, **2018**, *9*, 1–10.
51. Xue, L.-Y., et al. Reaxff-mpnn machine learning potential: a combination of reactive force field and message passing neural networks. *Phys. Chem. Chem. Phys.*, **2021**, *23*, 19457–19464.
52. Brough, D.B., Wheeler, D., Kalidindi, S.R. Materials knowledge systems in python—a data science framework for accelerated development of hierarchical materials. *Integr. Mater. Manuf. Innov.*, **2017**, *6*, 36–53.
53. Yang, Z., Yabansu, Y.C., Al-Bahrani, R., Liao, W.-K., Choudhary, A.N., Kalidindi, S.R., Agrawal, A. Deep learning approaches for mining structure-property linkages in high contrast composites from simulation datasets. *Comput. Mater. Sci.*, **2018**, *151*, 278–287.
54. Gupta, A., Cecen, A., Goyal, S., Singh, A.K., Kalidindi, S.R. Structure—property linkages using a data science approach: application to a non-metallic inclusion/steel composite system. *Acta Mater.*, **2015**, *91*, 239–254.
55. Cecen, A., Dai, H., Yabansu, Y.C., Kalidindi, S.R., Song, L. Material structure-property linkages using three-dimensional convolutional neural networks. *Acta Mater.*, **2018**, *146*, 76–84.
56. Yang, Z., Yabansu, Y.C., Jha, D., Liao, W.-K., Choudhary, A.N., Kalidindi, S.R., Agrawal, A. Establishing structure-property localization linkages for elastic deformation of three-dimensional high contrast composites using deep learning approaches. *Acta Mater.*, **2019**, *166*, 335–345.

57. Brough, D.B., Wheeler, D., Kalidindi, S.R. Materials knowledge systems in python—a data science framework for accelerated development of hierarchical materials. *Integr. Mater. Manuf. Innov.*, **2017**, *6*, 36–53.
58. Liu, R., Yabansu, Y.C., Agrawal, A., Kalidindi, S.R., Choudhary, A.N. Machine learning approaches for elastic localization linkages in high-contrast composite materials. *Integr. Mater. Manuf. Innov.*, **2015**, *4*, 1–17.
59. Liu, R., Yabansu, Y.C., Yang, Z., Choudhary, A.N., Kalidindi, S.R., Agrawal, A. Context aware machine learning approaches for modeling elastic localization in three-dimensional composite microstructures. *Integr. Mater. Manuf. Innov.*, **2017**, *6*, 160–171.
60. Piasecki, R. Microstructure reconstruction using entropic descriptors. *Proc. R. Soc. A*, **2010**, *467*, 806–820.
61. Li, X., Zhang, Y., Zhao, H., Burkhart, C., Brinson, L.C., Chen, W. A transfer learning approach for microstructure reconstruction and structure-property predictions. *Sci. Rep.*, **2018**, *8*, 13461.
62. Simonyan, K., Zisserman, A. Very deep convolutional networks for large-scale image recognition. 2014. arXiv: https://arxiv.org/1409.1556.
63. Gatys, L., Ecker, A.S., Bethge, M. Texture synthesis using convolutional neural networks. *Proceedings of Advances in Neural Information Processing Systems (NIPS)*, 2015, pp. 262–270.
64. Bostanabad, R., Bui, A.T., Xie, W., Apley, D., Chen, W. Stochastic microstructure characterization and reconstruction via supervised learning. *Acta Mater.*, **2016**, *103*, 89–102.
65. Grigoriu, M. Random field models for two-phase microstructures. *J. Appl. Phys.*, **2003**, *94*, 3762–3770.
66. Xu, H., Dikin, D.A., Burkhart, C., Chen, W. Descriptor-based methodology for statistical characterization and 3D reconstruction of microstructural materials. *Comput. Mater. Sci.*, **2014**, *85*, 206–216.
67. Butcher, J.B., Day, C.R., Austin, J.C., Haycock, P.W., Verstraeten, D., Schrauwen, B. Defect detection in reinforced concrete using random neural architectures. *Comput. Aid Civil Infrastruct.*, **2014**, *29*, 191–207.
68. Jang, K., Kim, N., An, Y.-K. Deep learning-based autonomous concrete crack evaluation through hybrid image scanning. *Struct. Health Monit.*, **2019**, *00*, 1–16.
69. Meredig, B., Agrawal, A., Kirklin, S., et al. Combinatorial screening for new materials in unconstrained composition space with machine learning. *Phys. Rev. B.*, **2014**, *89*, 094104.
70. Hautier. G., Fischer, C.C., Jain, A., Mueller, T., Ceder, G. Finding nature's missing ternary oxide compounds using machine learning and density functional theory. *Chem. Mater.*, **2010**, *22*, 3762–3767.
71. Saad, Y., Gao, D., Ngo, T., Bobbitt, S., Chelikowsky, J.R., Andreoni, W. Data mining for materials: computational experiments with AB compounds. *Phys. Rev. B.*, **2012**, *85*, 104104.
72. Guimaraes, G., Sanchez-Lengeling, B., Outeiral, C., et al. Objective-reinforced generative adversarial networks (ORGAN) for sequence generation models. arXiv: https://arxiv.org/1705.10843 [stat.ML].
73. Dai, M., Demirel, M.F., Liang, Y., Hu, J.-M. Graph neural networks for an accurate and interpretable prediction of the properties of polycrystalline materials. *npj Comput. Mater.*, **2021**, *7*, 1–9.

74. Hegde, V.I., et al. Reproducibility in high-throughput density functional theory: a comparison of aflow, materials project, and oqmd. 2020. arXiv: https://arxiv.org/abs/2007.01988.
75. Choudhary, K., et al. Computational scanning tunneling microscope image database. *Sci. Data*, **2021**, *8*, 1–9.
76. Khazanchi, D., Kumar Vyas, A., Kant Hiran, K., Padmanaban, S. *Blockchain 3.0 for sustainable development*. De Gruyter: Berlin, Boston, 2021. https://doi.org/10.1515/9783110702507.
77. Kant Hiran, K., Khazanchi, D., Kumar Vyas, A., Padmanaban, S. *Machine learning for sustainable development*. De Gruyter: Berlin, Boston, 2021. https://doi.org/10.1515/9783110702514
78. Vyas, A.K., Balamurugan, S., Kant Hiran, K., Dhiman, H.S. (Eds.). *Artificial intelligence for renewable energy systems*. John Wiley & Sons, 2022. ISBN: 9781119761693

CHAPTER 9

NATURE-BASED SMART MATERIALS (NBSMS): PROPERTIES, TYPES, AND APPLICATIONS

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ABSTRACT

The advantage of any application is based on the selection of nature-based smart biomaterials (NBSMs). These nature-derived smart biomaterials show several benefits in comparison to synthetic materials because these are biodegradable, biocompatible, recycled, and remolded in nature. The main target of this chapter is to present types, applications, and properties of NBSMs. NBSMs (biodegradable) made in nature are derived materials of biobased polymers. Recently, the production and utilization of NBSMs have increased to gain sustainability. These materials give the chance to overcome the major problem of pollution. Its mechanical strength, scaffold architecture, lightweight, durability, low cost, and chemical resistance power have increased its demand. NBSMs have a very huge market and a broad range of applications. These degradable NBSMs play an important part in every aspects of life as well as economy all over the world due to their excessive use in food packaging, agriculture, medical, construction, pharmaceutical, cosmetic industry, and defense. Bioplastics have many industrial applications due to which its consumption in this year (2021–2022) is 2.75 million tons.

9.1 INTRODUCTION

Smart materials are also known as advanced materials. These materials are capable to respond with external environments or exogenous stimuli under specific conditions. These accurate environmental conditions include strength, thermal, chemical, moisture, pH, light, magnetic field, and pressure [1, 2]. Some synthetic smart materials have a few disadvantages due to their composition, structure is not compatible with living tissues or organs, they do not show more affinity with living organisms remodeling. Nowadays, so many biomaterials have been developed to overcome the problems of synthetic materials [3]. Natural biomaterials can be divided in several groups according to their occurrence. Due to the responsive nature of environmental features these advanced biomaterials are widely used in a very broad range with full potential in different applications in self-sustainable wireless sensors, harvesting devices, biomedical devices, aeronautical equipment, defense, and construction industry [4, 5].

NBSMs have become an area of great interest in industrial sector due to their unique features and potential applications. The unique properties and various applications of the biopolymeric smart materials have made them a promising area of the research and development department. These materials are closer than ever to conventional smart materials. NBSMs are renewable resource-based biopolymers like alginate, gelatin, starch, chitosan, cellulose, silk, and so on have sufficient strength to rule over synthetic materials in industrial applications [6]. The NBSM market is expected to grow $6.12 billion by 2023 (according to market and market annual reports). NBSMs have very charming and multidisciplinary properties. This helps to improve the human condition and standard of living [7].

9.1.1 TYPES OF SYNTHETIC SMART MATERIAL

Synthetic smart materials are materials that can change their properties and nature in exposure to external stimuli such as temperature, light, magnetic fields, or electrical fields. Various types of synthetic materials include the following.

9.1.1.1 SHAPE MEMORY SMART MATERIALS

Shape-memory NBSMs are capable to regain their original shape after deformation. This phenomenon is mostly found in material that shows a reversible phase transition. This effect can be divided into two categories: first is the one-way shape memory effect and the second is the two-way shape memory effect. In the first one, the shape memory effect the material can regain only one predefined shape and in the two-way shape memory effect, the material can regain a multitudinous shape after deformation. These smart materials remember their original shape. These smart materials exhibit pseudo elasticity [8].

9.1.1.2 THERMO CHROMIC SMART MATERIALS

In this type of smart materials, NBSMs can alter their color or ocular properties in the presence of temperatures. In this type of materials, color change occurs due to shift in the equilibrium among the color former and color developer components of the mixtures [9, 10].

9.1.1.3 SMART PIEZOELECTRIC MATERIALS

Piezoelectric smart materials generate electricity on applying a mechanical stress. Recently, scientist shows the interest on these materials and their application in biomedical devices due to their biocompatible and biodegradable nature. Smart piezoelectric materials are used in medical equipment like sensor, actuators to convert flow rate and pressure [11].

9.1.1.4 PHOTO CHROMIC SMART MATERIALS

These smart materials can change color reversibly in exposure with irradiations. The major applications of photo chromic materials are depend on erasable/rewritable quality, high resolution, and high sensitivity [12].

9.1.1.5 MAGNETO RHEOLOGICAL SMART MATERIALS

Magneto rheological smart materials are a very alternative class of materials that show commanding changes in their properties when exposed to external stimuli. When a magnetic field is applied to these materials the ferrous materials align themselves along the field lines, which cause a change in materials stiffness and viscosity. The quasi-static model provides a simplified presentation of the matrix behaviors focusing on its response to mechanical or magnetic forces along a single direction. These materials can be used in the protection of buildings and bridges from storms and earthquakes [13, 14].

9.2 NATURE-BASED SMART MATERIALS

NBSMs are derived materials from living organisms like plants, algae, animals, fungi, and bacteria. Study on NBSMs has always been a topic of research and interest in academics and industries. Smart biomaterials (SBMs) are made by designing or incorporating peptide, protein, and other required functional groups into a polymeric chain (pictorial representation is shown in Figure 9.1) [15, 16].

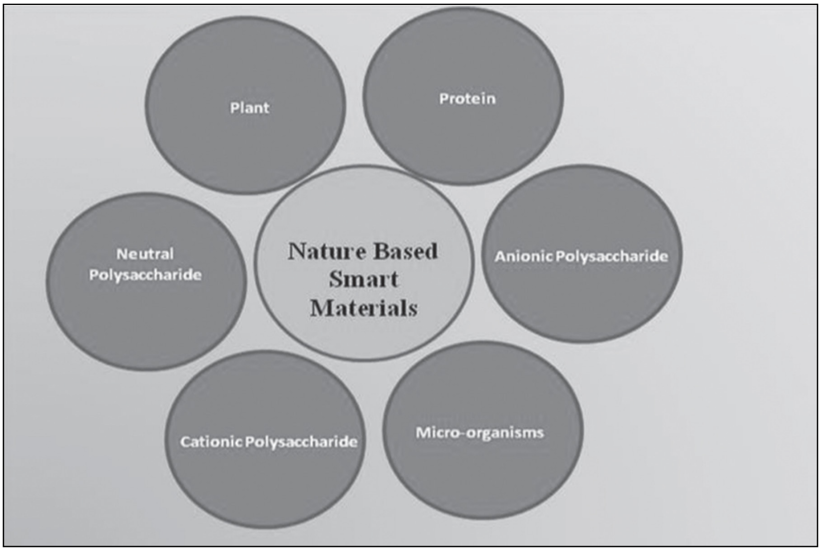
Plant
Protein
Neutral Polysaccharide
Nature Based Smart Materials
Anionic Polysaccharide
Cationic Polysaccharide
Micro-organisms

FIGURE 9.1 Pictorial representation of nature-based biopolymer sources. ⏎

9.2.1 NEED FOR NBSMS

Research on nature-based smart biopolymeric materials can be a very promising alternative to conventional synthetic plastic materials. These NBSMs are made from sustainable and ecofriendly components. The use of NBSMs leads the alertness of sustainability, pollution control, and proper decomposition of solid waste materials in the environment. Many bioplastics are widely used in our daily needs; out of all, we will discuss some commonly used bioplastics with their application [17].

9.2.1.1 STARCH

It is the main component of digestible carbohydrates. It is the most useful bioplastic that has been continuously used in several applications [18]. Starch is the main source of our diet, commonly found in plants. It is a simple molecule composed of glucose residues which are linked together by α-1,4-linkages and functions as an energy carrier in plants [19]. The internal arrangement of each chain of monomers may be unique to each plants, as shown in Figure 9.2. Starch is white, granular, and crystalline in structure. Its degradation is initiated by the hydrolysis of glycosidic bonds. The enzyme α-amylose starts the cleavage of long-chain starch molecules into small fragments of starch [20]. Starch is degraded by hydrolysis of glycoside linkage by a group of enzymes that accelerates the hydrolysis. α-Amylase starts the cleavage of a long polymeric chain of starch and creates monomers of starch [21]. These monomeric units are hydrolyzed by β-amylose, α-glucosidase, and glucoamylose. Fungus *Aspergilus oryzae* and bacteria *Bacillus stearothermophilus* produce a variety of enzymes for the degradation of starch; these enzymes are present in different types of soil. Gelatinization is the process that makes starch more susceptible for biodegradation. During gelatinization, starch is dissolved in water at high temperatures and loses its original granular shape by breaking intermolecular hydrogen bonds [22].

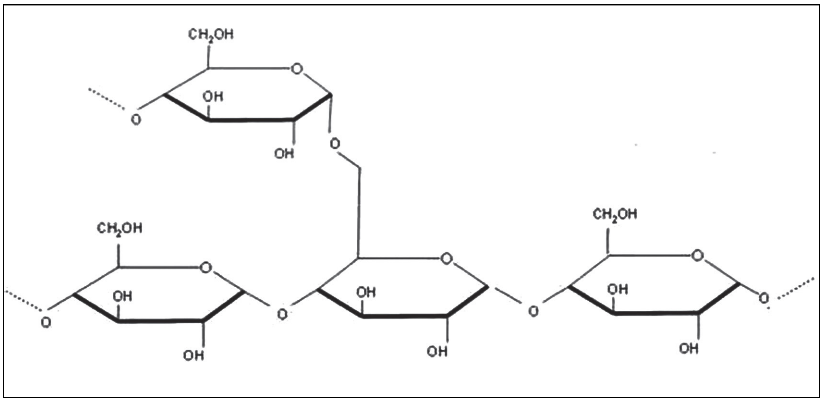

FIGURE 9.2 Structure of starch.

9.2.1.2 CARBOXY METHYL CELLULOSE

Carboxy methyl cellulose (CMC) is the most abundant and a prime cellulose derivative. It is a water soluble, cheaper, and nontoxic heteropolysaccharide obtained from cellulose [23]. CMC possesses higher mechanical strength, promising biocompatibility, biodegradability, and low inflammability that make it an ideal material for pharmaceutical, agriculture, and construction industries [24]. CMC is a fully degraded polysaccharide and can be degraded completely in environmental systems such as rivers and soils. It does not produce any toxic side product during degradation. Cellulase enzymes are responsible for the degradation of cellulose by the hydrolysis of β-1,4-linkages [25]. Cellulase enzyme system consists of three types of soluble extracellular enzymes. 1,4-β-Endoglucanose, 1,4-β-exoglucanose, β-glucosidase, β-1,4-glycosidic bonds of cellulose chains cleavage are initiated by endoglucanose (Figure 9.3). Cleavage of cellulose into glucose involves a series of enzymatic reactions. This process starts with the initialization of exoglucanoses, which breakdown the nonreducing ends of the cellulose chain. Exoglucanoses are enzymes that break the β-1,4-glycosidic bonds at the ends of the cellulose chains, releasing cellobiose units [26].

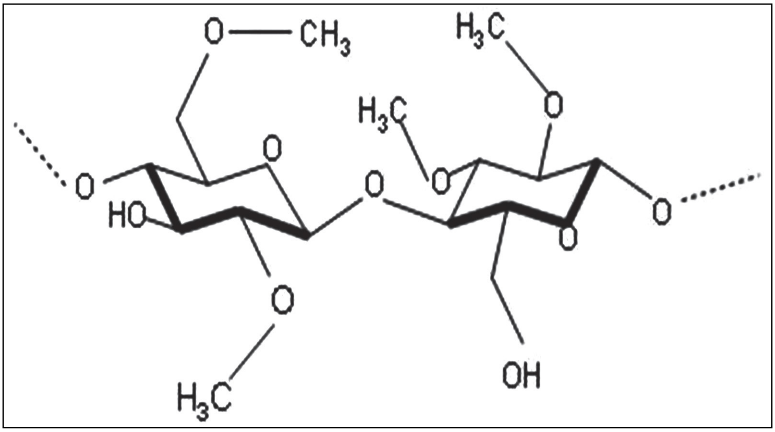

FIGURE 9.3 Structure of carboxy methyl cellulose (CMC). ⏎

9.2.1.3 GELATIN

Gelatin is a biodegradable, biocompatible, cheap, ecofriendly, nontoxic, and noncarcinogenic biopolymer and it is one of the widely used bioplastics with animal proteins [27]. Gelatin is extracted is from partial hydrolysis of collagen and also found in animal protein. Collagen consists of all 20 amino acids in its three α-chains; these chains are stabilized and interlaced by hydrogen bonds into a triple helix with clockwise rotation, as depicted in Figure 9.4 [28]. Collagen may be synthesized by two pretreatments, acid and alkali, which gives type A and type B gelatin, respectively. Gelatin has been utilized in the gelatin process [29]. Gelatin is highly applicable in medical science and as a smart packaging material because it dissolves quickly in an aqueous environment. Gelatin can be used as a promising bioplastic in the plastic world. As a single compound, it is hydrophilic in nature with very weak tensile strength. Gelatin's high ability of degradation makes it important in industrial applications [30].

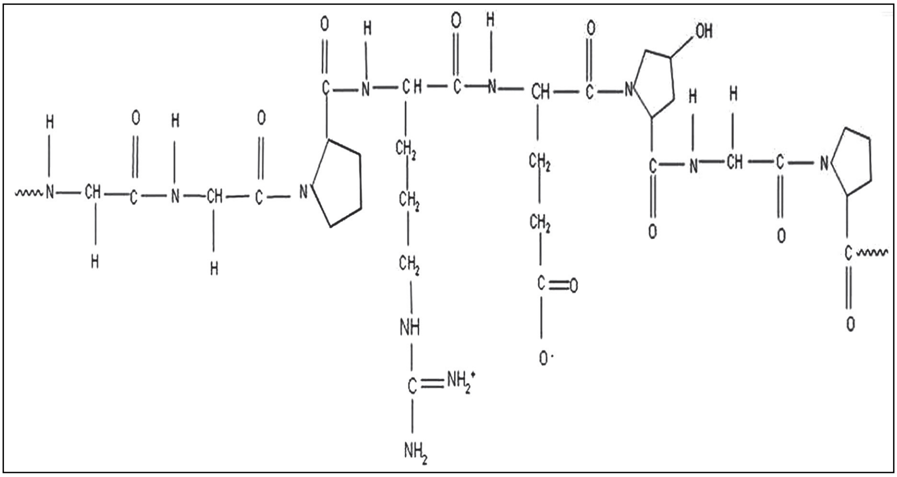

FIGURE 9.4 Basic chemical structure of gelatin. ⏎

9.2.1.4 ALGINATE

Alginate is indeed an anionic polysaccharide that is extracted from the cell walls of brown algae, including *Macrocystis pyrifera*, *Laminaria hyperborean*, and *Ascophyllum nodosum*. Alginate is widely used in many foods and biomedical applications due to its biocompatibility, low toxicity, and biodegradable nature. Alginates are linear chain bioplastics consisting 1,4-linked β-D-mannuronic acid (M) and 1,4-α-L-guluronic acid (G) residues, as shown in Figure 9.5 [31]. The extraction method of alginate is simple. Alginate is commercially available in different grades of molecular weight and composition. Alginate is environmentally degraded by alginate lyases or depolymerases. Alginate lyses are extracted from marine microorganisms and marine animals. The cell wall of brown algae is a major source of alginate lyses enzyme. It is alginate rich and natural source of carbon and energy. Degradation cleavage is initiated by β-elimination of the polymeric chain. The maximum number of lyases enzymes are involved in endolytic cleaving reactions; only a few are available for exolytic activity. According to Gacesa, this degradation follows three steps: (1) removal of negative charge on the carboxyl anion, (2) abstraction of the proton on C5 by a general base-catalysis; and (3) transfer of electron from carboxyl group to form a double bond between C4 and C5, resulting in the β-elimination of the 4-*O*-glycosidic bond [32]. Alginate lyases are generally used in the study of alginate, but they take an active part biofuel production [33].

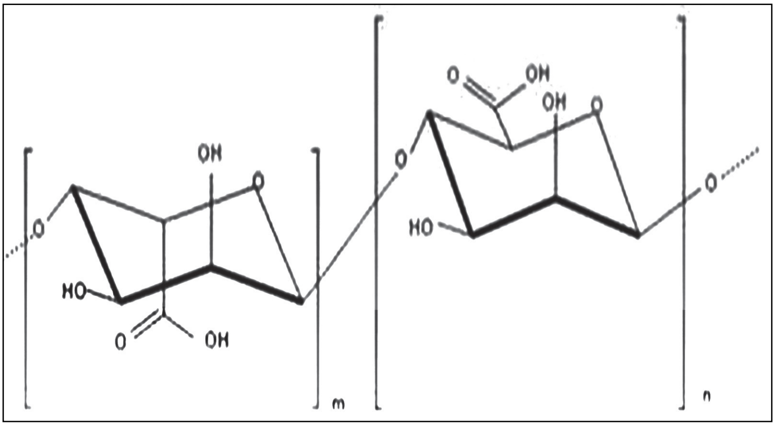

FIGURE 9.5 Molecular structure of alginate.

9.2.1.5 LIGNIN

Lignin is one of the most frequently used resources for bioplastic production, because of its huge abundance in nature. Lignin is a class of hydrocarbon polymers consisting aliphatic and aromatic structures (Figure 9.6) [34]. It has three-dimensional amorphous polymeric structures, which contain high molecular weight with phenyl propane units. It is a coproduct of paper and pulp industries. Lignin works as a binding agent to bind the separated fiber cells together as a natural cementing agent. Lignin is insoluble in most of the solvents; it cannot be fragmented into smaller units [35].

The amount of lignin content affects the morphology and properties of fibers. Lignin can be extracted from different lignocellulosic parts by applying chemical, biochemical, and physical steps. One of the most important properties of lignin is that it acts as an excellent UV-shielding material to replace synthetic absorbers. Lignin composite material can be used in food packaging, solar panel production, and medical science. The degradation mechanism of the lignin is not extensively described in the literature due to its insoluble nature, structural complexity, and lack of hydrolysable linkages. Therefore, it is difficult to explore efficient approaches to degradation by a chemical and physical ways. White rot fungi play an important role in the degradation of lignin [36].

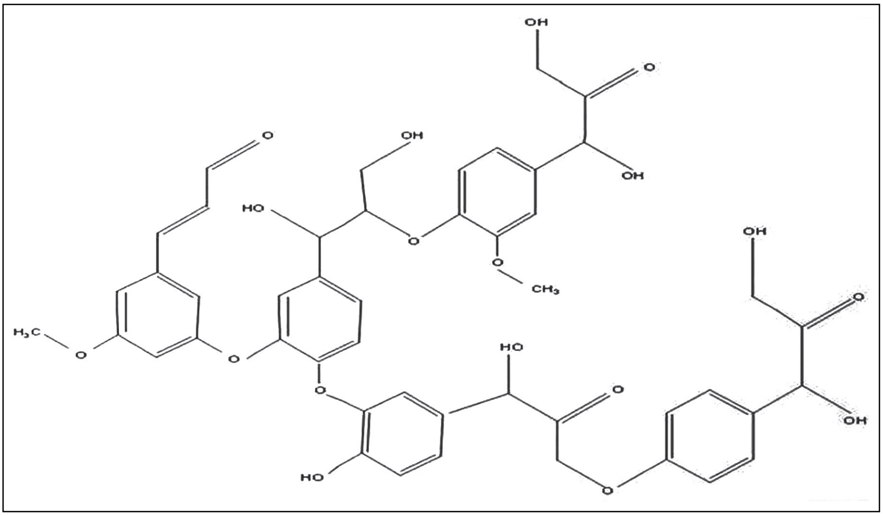

FIGURE 9.6 Chemical structure of lignin. ⏎

9.2.1.6 XANTHAN GUM

Xanthan gum is a fermented derivative product of renewable carbohydrates. These are easily degradable and environmentally safe. Its physicochemical properties make it a very constructive stabilizer for water-based systems, especially in cosmetic products. Its areas of applications cover a broad range from the food industry to oil drilling, polishes, and agricultural flowable, as mentioned in Figure 9.7 [37].

In the food industry, it is used as sauces, gravies, dairy products, low-calorie food, and salad dressings. It is also used as a suspending agent. A recent research showed that xanthan gum improves the strength of soil, especially in the presence of clay particles, due to hydrogen bonding between xanthan gum and clay particles [38]. Xanthan gum is composed of a repeating unit of D-glucose, D-mannose, and D-guluronic acid in the molar ratio of 2:2:1 [39]. The primary structure of xanthan gum is linear (1–4)-linked β-D-glucose, a backbone with a trisaccharide side chain on every other glucose at C-3 containing a glucoronic acid residues linked (1–4) to a terminal mannose unit and (1–2) to a second mannose that connects to the backbone, being as natural and highly stable polysaccharide. It is degradative parts are oligosaccharides, monosaccharides, water, and carbon dioxide. The degradation of xanthan is started by an enzymatic attack by the secration of xanthanase (endo-β-D-glucanase) and xanthan lyase. The rate of xanthan degradation depends on the presence of microorganisms producing relevant enzymes and environmental conditions [40].

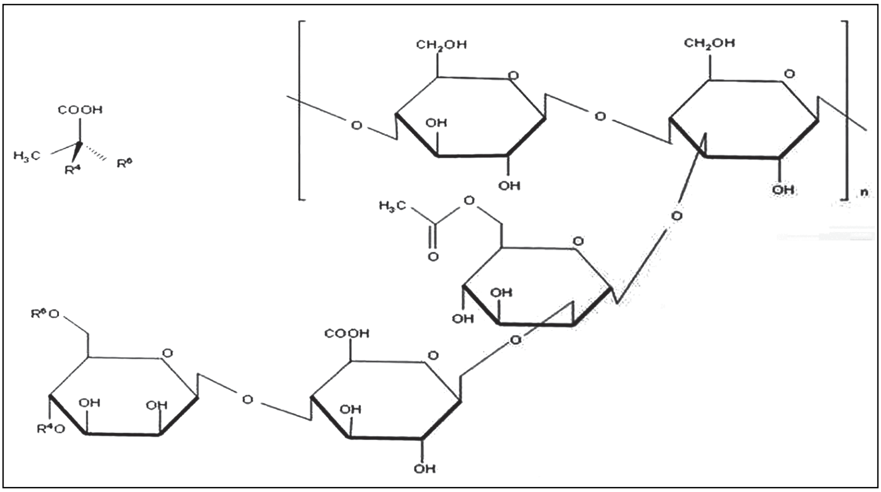

FIGURE 9.7 Chemical structure of xanthan gum. ⏎

9.2.1.7 CHITOSAN

Chitosan is the second most plentiful and renewable polysaccharide in the world, that is, derived from chitin. Chitosan is produced from the shells of molluskan, it has some very remarkable properties like molecular weight, degree of acetylation, degree of crystallinity; due to all these features, it is used in food and packaging, paper and pulp, agriculture, cosmetic, textile, aerospace, and beverages industry [40]. Chitosan is indeed a linear polysaccharide composed of repeating units of β-(1–4)-linked 2-amino-2-deoxy-β-D-glucopyranose and 2-acetamido-2-deoxy-β-D-glucopyranose residues (as shown in Figure 9.8). Its low degree of acetylation helps to degrade easily.

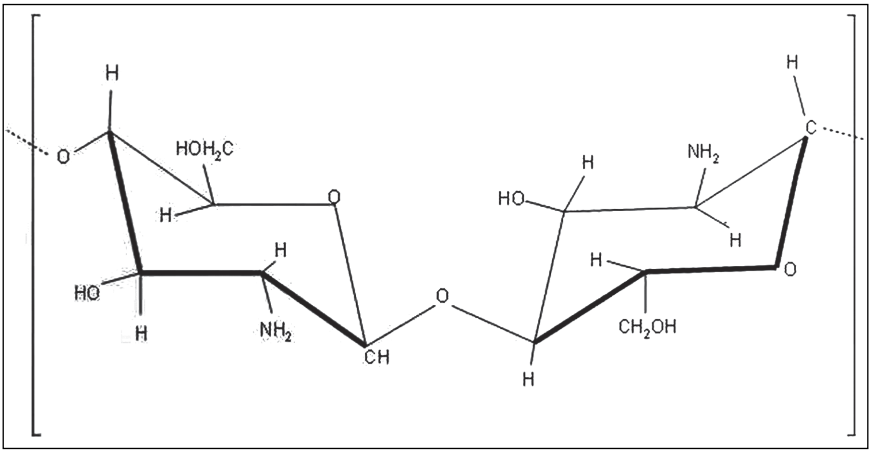

FIGURE 9.8 Chemical structure of chitosan. ⏎

Chitosan degradation is based on the distribution of acetamide groups in the chitosan molecular chain. The degree of acetylation affects the viscosity of chitosan solution. The molecular weight of chitosan molecule is very important for the degradation because it changes from 300 to over 1000 kDa [41–43].

9.2.1.8 SILK

Silk is a structural animal protein, which represents a very specific, ancient class of biocompatible, and easily processed biopolymer. Silks are fibrous proteins which are produced within glands after biosynthesis in epithelial cells in silkworms and spiders. Bombycidae and saturniidae are well-known species of silkworm. Currently, regenerated silk solutions have been used to form lots of SBMs due to their high mechanical, structural, and biological properties. Silk is made up of two components—silk fibroin (SF) and silk sericin. Natural silk contains long molecular chains due to the presence of long amino acid chains (Figure 9.9) [44].

Lower molecular weights of SF can be made by processing silk. Natural silk is used in medication of cystitis, impotence, cancer, edema, and so on.

Silk protein derivative is used as antiinflammatory agent, antitumefacient agent, dressing material and in several dentistry applications. Silk is used as tissue regeneration for wound healing. SF plays a very important role in cosmetic industries due to its flexible, glossy, crystalline, spreading, and adhesive characteristics [45].

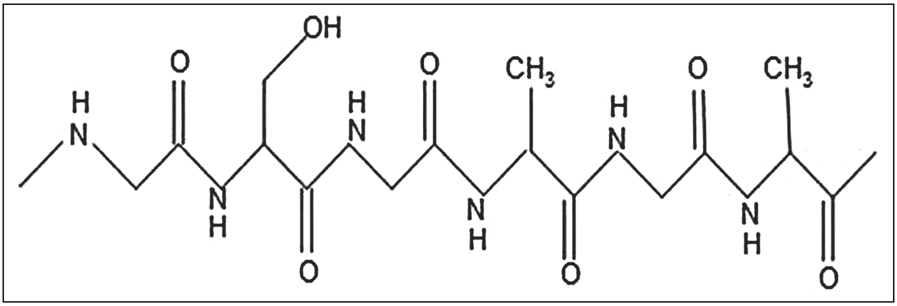

FIGURE 9.9 Chemical structure of silk. ⏎

9.3 NBSMS APPLICATION IN DIFFERENT SECTORS

9.3.1 NBSMS IN FOOD PACKAGING APPLICATIONS

Food is an essential need for survival. The increasing demand for high food quality, quantity, hygiene, and nonpolluting waste products are the common needs that have been encouraging scientists to search the NBSMs, which gives new challenges and opportunities for the preparation of NBSMs in food industry. To stipulate drawing on eco-friendly material for packing according to a green environmental approach is now become a major challenge for industries. Since nonbiodegradable packaging has issue of disposal associated with it, industrialists have to consume their major earnings on treatment before dumping. The untreated packing disposes accumulate within soil and water and may contaminate the environment causing pollution, toxicity, and a rise in Earth's temperature. Therefore, perishable or recyclable form of packaging materials is introduced as an alternative [46, 47]. Nowadays, carbohydrates, protein, and nanooxide metal particles are used in biodegradable packaging along with nanoclays [48]. These types of NBSMs show great advantageous properties due to their ecofriendly nature, biodegradability, bioavaility, nontoxicity, renewability, high strength, and ductibility. In recent years, nature-based polymers have been found to have been various applications in packaging applications. In the food industry, biopolymers are used in the form of edible films, coating, jelly, and so on. Food packaging is one of the most beneficial steps to maintain the hygiene and quality of food products for storage, transportation, and enduse [49]. Yaradoddi et al. [50] developed a biodegradable packaging material for sustainable packaging material using CMC. The main purpose of this research work was to convert the agricultural waste material to important biologically degradable polymeric material for packaging purposes. In this process, sugarcane bagasse was used to prepare low-cost film with other biopolymers like gelatin and agar with variations of glycerol concentration. Fourier transform infrared spectroscopy, differential scanning calorimetry, and WP analytical techniques were used to characterize the prepared biodegradable sample. It was noticed that the prepared sample was very good in mechanical strength and effectively compatible with the soil burial method. Sulfur nanoparticles (SNPs) were prepared with calcium crosslinking and alginate biopolymeric smart material in different concentrations for the study of functional properties by Priyadarshi et al. [51]. The results reveal the additional use of SNPs showed supertensile strength and water vapor barrier properties. Results reveal the penetration of SNPs enhanced the hydrophobicity of the film, which increased the water contact angle and decreased the moisture content of the prepared film, as shown by the TGA. Thus, the alginate and SNP composite film may be the best substitute for the packaging of frozen foods with high moisture content. Costa et al. [52] discovered the films to be used as active pads for meat packages to increase their shell-life for preservation. In different variations, chitosan and cellulose nanocrystals were tested on the prepared films by the solvent casting process. Several spectral analyses have been carried out to check the quality and efficiency of the developed film. Results prove that the antimicrobial nature, transparency, and mechanical properties were enough to enhance the food shelf life.

9.3.2 NBSMS IN CONSTRUCTION TECHNOLOGY

In the present scenario, various biopolymeric smart materials are available with customized features. Nowadays, smart biopolymers are widely used in construction technologies. Biopolymers are appropriate construction materials because these are cheap, ecofriendly, and easily available with good mechanical strength in nature. The advanced biopolymer-based formulations are discovered by utilizing several types of reinforcements such as nanoparticles, synthetic fibers, and natural fibers [53].

Roll of smart materials in the construction and architecture industry:

- To improve the strengths and toughness of concrete.
- Protection from UV radiation.
- In small amounts, nanomaterials improve reinforcing of steel regarding corrosion and deterioration.
- To produce water filters purifiers and treatment systems.
- In the production of advanced photovoltaic cells and panels.
- Waterproofing materials, paints, glues, sealants, telecommunication, and illumination electronic parts are the most applicable materials which are used in construction technology [54].

Tourtelot et al. [55] synthesized the different biopolymers from various vernacular techniques to utilize and increase the compressive strength of the construction soil from the Paris region. The above researchers showed that cellulose-based fibers and wheat starch increase the compressive strength of the earth from 3.5 to 5.5 MPa and 4.5 MPa. Cellulose fibers and wheat starch were examined with clay. These SBMs applied as suitable material for use in construction technology in the present study and these are available as waste material from paper and pulp industry, agriculture, or agro-food-based industries. These biopolymers help in the development and preparation of construction using Earth-based building materials. The study conducted by Soldo et al. [56] focused on the use of various biopolymeric smart materials for improving soil strength. The researchers investigated the effects of xanthan gum, beta 1,3/1,6-glucan, guar gum, chitosan, and alginate on soil strength through different tests such as compression, splitting tensile, triaxial, and direct shear tests. They also examined the influence of different concentrations of these biopolymers and the duration of preservation on the test results. Additionally, the researchers exposed both untreated soil and biopolymer-treated specimens to real atmospheric conditions to evaluate their susceptibility to natural elements. The experimental findings indicated that the soil strength increased with higher concentrations of biopolymers and longer curing times. However, there was a point where the soil strength did not significantly change even with further increases in biopolymer concentration and curing time. Furthermore, the biopolymer-treated specimens exhibited better resistance to environmental conditions compared to untreated soil. Among the biopolymers tested, xanthan gum, guar gum, and beta-1,3/1,6-glucan demonstrated the strongest effect and showcased the promising potential for sustainable engineering applications. Overall, this study suggests that the use of biopolymeric smart materials can enhance soil strength and improve resistance to environmental influences. The specific biopolymers mentioned, namely, xanthan gum, guar gum, and beta-1,3/1,6 glucan, showed particularly promising results, indicating their potential for future applications in sustainable engineering.

9.3.3 NBSMS IN BIOMEDICAL

SBMs can be used as a very strong tool in biomedical applications, which acts as a control, constructed, and maintained dose at a molecular level of human as well as animal health by using engineered nanotechnical devices like nanodrugs and nanorobots. This success for biomaterials in the medical field totally depends on the devices and techniques. The great and beneficial properties of biopolymeric nanomedical devices are the nanosize which occupies very small surface to enter the human body in which the old and conventional medical devices cannot. Medical nanorobots are an example of the applicability of nanomedical devices, which can penetrate inside the human body through the very small blood vessels into any cavities inside the body. The possible applications of polymeric nanomedicines depend on technologies, materials, and instruments. SBMs can be used for fast diagnosis, rapid healing, and repair of genetic material, while nanomaterials and nanoinstruments are used as important aids in the treatment and transport of active ingredients [57].

Nature-based polymers have the ability of used for various biomedical applications by purpose of repair, fixation, bonding, covering, absorbability blockage, isolation, contact inhibition, cellular proliferation, and controlled and targeted drug delivery. NBSMs are used for various purposes in medical science: (1) It is used to replace nonfunctional or diseased tissues; (2) to help in the adjustment of tissue and ligament, tendon repair devices; and (3) to deliver drugs to different parts of the body in definite period of time. Chitosan is achieving attention in biomedical science due to its physicochemical properties and characteristics. Chitosan possesses multiple characteristics such as good mechanical strength, antimicrobial properties, biocompatibile nature, biodegradability, stimuli-responsiveness, and water solubility; due to all these characteristics features, Selvakumar Murugesan and Thomas Scheibel (2021) [58] prepared chitosan containing nanoparticles, nanovehicles, nanocapsules, scaffolds, fiber meshes, and 3D printed scaffolds for a variety of applications. In present time, chitosan-based nanoparticles have been identified to show biocompatibility as regenerative medicine in wound dressing, biosensors, and targeted drug delivery applications. According to Messmer [59], CMC is used in many treatments as lubricants, due to its fibrous nature and binding behavior to human corneal epithelial cells most probably through interaction with glucopyranose subunits and glucose transporters. SBMs can be used as a biomedicine, which acts as a control, constructed, and maintained dose at a molecular level of human as well as animal health by using engineered nanodevices, nanostructures, nanodrugs, and nanorobots. This success for biomaterials in the medical field lies in the ways and devices, which are, relies on this technique. The great and beneficial properties of biopolymeric nanomedical devices are their small size which takes very small space to enter the human body in which the traditional medical devices cannot. Surgical nanorobots are an example of the applicability of nanomedical devices, which can be introduced into the human body through the blood vessels or the ends of catheters into any cavities inside the body. The possible applications of polymeric nanomedicines depend on technologies, materials, and instruments. Smart biomaterials can be used for fast diagnosis, rapid healing, and repair of genetic material, while nanomaterials and nanoinstruments are used as important aids in the treatment and transport of active ingredients [60]. Recently, Pimentel and his colleagues [61] reported the fabrication of vascularized constructs using modified gelatin (transglutaminase-crosslinked gelatin) which is promising for the fabrication of complex tumor models. They concluded that gelatin could be considered as one of the promising and challenging biomaterials in future prospects. The field of SBMs, which encompasses materials that promote the repair, replacement, or restoration of hard and soft tissues, has witnessed significant growth as the global population continues to age. Traditionally, SBMs have been defined as those capable of responding to stimuli. Montoya et al. [62] reported up-to-date applications of SBMs for hard tissues, based on the materials' responses (external and internal stimuli) and their properties as immune-modulatory biomaterials.

9.3.4 NBSMS IN AGRICULTURE

The worldwide population is growing day by day; therefore, food production, distribution, and security is a major problem for all of us. The agriculture industry is one of the most significant waste-producing sectors, with a large amount of production processing waste. The agricultural sector is facing a diverse issue due to the overconsumption of land; it causes the loss of soil fertility, forage, and crop yield. New agricultural techniques have become more beneficial for enhancing the crop yield. However, these modern technologies have an adverse effect and create long-lasting footprints in the environmental, health, social, and economic sectors [63]. Danila Merino and coworkers [64] prepared the sprayable mulch suspension with the use of sodium alginate and three different concentrations of seawood *Undaria pinnatifida* microparticles. The whole treatment was carried out in tomato plants, including polyethylene as a control treatment. At the end of aerial fresh and dry weights, chlorophyll content, green canopy cover, anthomycin contents were determined in tomato plants. Results showed that the developed alginate-rich mulches are very useful nutritional products for substrate and plants. The application of agrochemicals and biological agent-loaded microparticles plays a very important role for the protection, production, and controlled release of fertilizer and agrochemicals. Parente et al. [65] discovered ways to improve scientific research and industrial processes. Recently, scientists suggested that biopolymers are the most powerful solution for synthetic microcapsule systems. Safety, efficiency, biocompatibility, nontoxicity, and biodegradability are some of the important properties that can biodegrade polymeric matrix under climatic and lab conditions. The controlled and targeted release of encapsulated active agents is a research field that, over the years, has been constantly innovating due to the promising applications in the areas of pharmaceutical, agriculture, cosmetic, and textile industries. Gelatin is an effective biostimulant. It can provide nitrogen that enhances plant growth. Wilson and coworkers [66] provided information that gelatin is an animal protein. It is very much effective for plant growth. Lopez-Velazquez et al. [67] prepared a chitosan, gelatin, and polyvinyl alcohol hydrogel to increase the substratum water-absorbing capacity, improve soil structure, and control the release of inulin (agrochemicals) to enhance protection in chilli plant against *Phytophthora capsici*. The hydrogels showed a dense, interconnected, tridimensional, and reticulated structure, which shows the penetration of inulin inside the hydrogel.

9.3.5 NBSMS IN COSMETIC INDUSTRY

The applications of SBMs in cosmetics manufacturing is indicative of the large potential technology, which represents the cosmetics industry. Varieties of NBSMs are already in use in cosmetic applications.

The biomaterials are used as encapsulated material vehicles for delivery of active agents.

1. NBSMs in the form of nanostructure reduce direct interaction of strong sensitive agents with skin.
2. NBSMs delayed the release of sensitizing agents.

3. Reduces the amount of agents and additives.
4. Increased longer released time of active ingredients and hence greater product acceptability.

Cosmetics composed of biopolymers show an effective design, with advantages of their thermal and chemosensitive properties. Cosmetic biomaterials are also used for the making of nanoparticles for the delivery of, for example, fragrances. The use of natural biopolymers in cosmetic formulations is of particular relevance because of their biocompatible, safe, nontoxic, and eco-friendly character. These formulations are highly attractive and marketable to consumers and are suitable for several applications, including skin, hair makeup, oral care, and as modifiers and stabilizers [68]. Alina Sionkowska with coworkers [69] prepared the film of fish skin collagen and chitosan. They characterized the features of the film by infrared spectroscopy, mechanical properties study, contact angle measurements, topographic imaging, and swelling test techniques. Hydrophilicity and polarity of the film decrease with the increasing collagen content, which may suggest that the adhesion to the skin will be enhanced.

9.3.6 SMART BIOMATERIALS IN DEFENSE

Defense technology demands include not only efficiency and security, yet also the material applied. The intensification in research of biomaterials in a few years occurred primarily due to their attractive potential in mechanical and physical properties. Defense is an important area where SBMs are applied. Biomaterials in defense help to maintain fuel economy, soldier safety, stealth movement, food storage, packing material for security, counterfeiting safety and microbial purpose, use and types of antibacterial paper, water filter, tissue paper, helmet designs, light-weighed army vehicles, intelligent, or smart coating or aircraft materials.

According to Higgs [70], nature-based packaging materials in the military are generally used to protect food items, beverages, electronics, electrical, and machinery parts. For all these purposes, biopolymeric nanocellulose can be used in the form of bags, cartons, tapes, wraps, and so on. Nayak et al. [71] stated that cellulose-based bioformulations like nanocellulose can be used in electronic textiles to monitoring personnel health, their blood pressure, heartbeat, body temperature, location of defense, for communications, and for environmental temperature monitoring. The applications of nanocellulose have promptly made these textile materials good conductive agents in defense.

Nechyphorchuk et al. [72] developed woven cotton fabrics using CNF (cellulose nanofibers) mixed with plasticizers applicable for printing or dyeing. These fabrics are continuously used for as conventional colored water-based inks and conductive silver nanoparticle inks. These CNF helped the inks to set onto the surface of the substrate, which gives best quality with faster printing speed production. These CNFs make a conductive layer, which arrange their electric signal even when being folded.

9.4 CONCLUSION

Nowadays, NBSMs are an intrinsic part of our society. NBSMs can allow living beings to live longer and healthier because these materials have sufficient ambidexterity nature to handle some dangerous diseases. Industrial interest and belief in NBSMs have constantly increased over the decades. These materials are closer than ever to conventional smart materials. NBSMs are renewable resource-based biopolymers like alginate, gelatin, starch, chitosan, cellulose, silk, and so on have enough strength to rule over synthetic materials in industrial applications. The NBSMs market is expected to grow $6.12 billion by 2023 (according to markets and market annual report). In this chapter, we have given an overview of the NBSMs' properties, application, structure, and types.

KEYWORDS

- **NBSMs**
- **properties**
- **structure**
- **applications**
- **classification of biomaterials**

REFERENCES

1. Bril, M., Fredrich, S., Kurniawan, N.A. Stimuli-responsive materials: a smart way to study dynamic cell responses. *Smart. Mater. Med.*, **2022**, 257–273.
2. Chakrapani, G., Zare, M., Ramakrishna, S. Intelligent hydrogels and their biomedical applications. *Mater. Adv.*, **2022**, *3*, 7757–7772.

3. Bhargava Reddy, M.S., Ponnamma, D., Choudhary, R., Sadasivuni, K.K. A comparative review of natural and synthetic biopolymer composite scaffolds. *Polymers*, **2021**, *13*(7), 1105.
4. Troy, E., Tilbury, M.A., Power, A.M., Wall, J.G. Nature-based biomaterials and their application in biomedicine. *Polymers (Basel)*, **2021**, *13*(19), 3321.
5. Ensieh, S., Hosseini, E.S., Dervin, S., Ganguly, P., Dahiya, R. Biodegradable materials for sustainable health monitoring devices. *ACS Appl. Bio. Mater.*, **2021**, *4*(1), 163–194.
6. Basim, P., Gorityala, S., Kurakula, M. Advances in functionalized hybrid biopolymer augmented lipid-based systems: a spotlight on their role in design of gastro retentive delivery systems. *Arch. Gastroenterol. Res.*, **2021**, *2*(1), 35–47.
7. Hartmann, F., Baumgartner, M., Kaltenbrunne, M. Becoming sustainable, the new frontier in soft robotics. *Adv. Mater.*, **2021**, *33*(19), 1–32.
8. Mu, T., Liu, L., Lan, X., Liu, Y., Leng, J. Shape memory polymers for composites. *Compos. Sci. Technol.*, **2018**, *160*, 169–198.
9. Nawade, A., Ramya, K., Mukhopadhyay, S. *Design, process, implementation and recent developments. Energy saving coating materials,* 2020, pp. 197–226.
10. Wang, X., Narayan, S. Thermochromic materials for smart windows. A state-of-art review, *Sec. Solar Energy*., **2021**, *9*, 1–6.
11. Jacob, J., More, N., Kalia, K., Kapusetti, G. Piezoelectric smart biomaterials for bone and cartilage tissue engineering. *Inflamm. Regener.*, **2018**, *38*(2), 1–11.
12. Leistner, A.L., Pianowski, Z.L. Smart photochromic materials triggered with visible light. *Eur. J. Org. Chem.*, **2022**, *19*, 1–20.
13. Ahamed, R., Choi, S-B., Ferdaus, M.M. A state of art on magneto-rheological materials and their potential applications. *J. Intell. Mater. Syst. Struct.*, **2018**, *29*(10), 2051–2095.
14. Vicente, J.D., Klingenberg, D.J., Hidalgo-Alvarez, R. Magnetorheological fluids: a review. *Soft matter*, **2011**, *7*(8), 3701–3710.
15. Khan, F., Tanaka, M. Designing smart biomaterials for tissue engineering. *Int. J. Mol. Sci.*, **2018**, *19*(1), 17, 1–14.
16. Zhang, H., Wu, X., Quan, L., Ao, Q. Characteristics of marine biomaterials and their applications in biomedicine. *Mar. Drugs.*, **2022**, *20*(372), 1–32.
17. Katiyar, N.K., Goel, G., Hawi, S. et al. Nature-inspired materials: emerging trends and prospects. *NPG. Asia. Mater.*, **2021**, *13*(56), 1–16.
18. Ali, M.I., Ahmed, S., Javed, I., Ali, N., Atiq, N., Hameed, A., Robson, G. Biodegradation of starch blended polyvinyl chloride films by isolated Phanerochaete chrysosporium PV1. *Int. J. Environ. Sci. Technol.*, **2014**, *11*, 339–348.
19. Smirnova, J., Alisdair, F., Steup, M. Starch: metabolism and structure. *Starch Degrad.*, **2015**, 239–290.
20. Muthukumar, T., Aravinthana, A., Dineshram, R., Venkatesan, R., Doble, M. Biodegradation of starch blended high density polyethylene using marine bacteria associated with biofilm formation and its isolation characterization. *J. Microb. Biochem. Technol.*, **2014**, *6*, 1–7.
21. Schlemmer, W., Selinger, J., Andreas, M., Spirk, H.S. Polysaccharides for sustainable. energy storage-a review. *Carbohyd. Polym.*, **2021**, *265*(118063), 1–16.
22. Asatsuma, S., Sawada, C., Itoh, K., Okito, M., Kitajima, A., Mitsui, T. Involvement of α-Amylase I-1 in starch degradation in rice chloroplasts. *Plant. Cell. Physiol.*, **2005**, *46*(6), 858–869.

23. Karimi, M., Naimi-Jamal, M.R. Carboxymethyl cellulose as a green and biodegradable catalyst for the solvent-free synthesis of benzimidazoloquinazolinone derivatives. *J. Saudi. Chem. Soc.*, **2019**, *23*, 182–187.
24. Miehle, E., Bader-Mittermaier, S., Schweiggert-Weisz, U., Hauner, H., Eisner, P. Effect of physicochemical properties of carboxymethyl cellulose on diffusion of glucose. *Nutrients*, **2021**, *13*(5), 1398, 1–18.
25. Wiwatwongwana, F., Surin, P. In Vitro degradation of gelatin/carboxymethylcellulose scaffolds for skin tissue regeneration. *Chem. Eng. Trans.*, **2019**, *74*, 1555–1560.
26. Shim, E., Noro, J., Cavaco-Paulo, A., Silva, C. Carboxymethyl Cellulose (CMC) as a template for laccase-assisted oxidation of aniline. *Front. Bioeng. Biotechnol.*, **2020**, *8*, 1–13.
27. Baranwal, J., Barse, B., Fais, A., Delogu, G.L., Kumar, A. Biopolymer: a sustainable material for food and medical applications. *Polym*, **2022**, *14*, 983, 1–22.
28. Jafari, H., Lista, A., Siekapen, M.M., Ghaffari-Bohlouli, P., Nie, L., Alimoradi, H., Amin, S. Fish collagen: extraction, characterization, and applications for biomaterials engineering. *Polymers*, **2020**, *12*, 2230, 1–36.
29. Rodsuwan, U., Thumthanaruk, B., Kerdchoechuen, O., Laohakunjit, N. Functional properties of type A gelatin from jellyfish (*Lobonema smithii*). *Int. Food. Res. J.*, **2016**, *23*, 507–514.
30. Nur Hanani, Z.A., Roos, Y.H., Kerry, J.P. Use and application of gelatin as potential biodegradable packaging materials for food products. *Int. J. Biol. Macromol.*, **2014**, *71*, 94–102.
31. Martau, G.A., Mihai, M., Vodnar, D.C. The use of chitosan, alginate, and pectin in the biomedical and food sector—biocompatibility, bioadhesiveness, and biodegradability. *Polymers*, **2019**, *11*, 1837, 1–28.
32. Zhang, Y.H., Shao, Y., Jiao, C., Yang, Q.M., Weng, H.F., Xiao, A.F. Characterization and application of an alginate lyase, Aly1281 from marine bacterium *Pseudoalteromonas carrageenovora* ASY5. *Mar. Drugs.*, **2020**, *18*(2), 95.
33. Guarino, V., Caputo, T., Altobelli, R., Ambrosio, L. Degradation properties and metabolic activity of alginate and chitosan polyelectrolytes for drug delivery and tissue engineering applications. *AIMS Mater. Sci.*, **2015**, *2*(4), 497–502.
34. Souza, R.E., Gomes, F.J.B., Brito, E.O. et al. A review on lignin sources and uses. *J. Appl. Biotechnol. Bioeng.*, **2020**, *7*(3), 100–105.
35. Gheorghita, R., Anchidin-Norocel, L., Filip, R., Dimian, M., Covasa, M. Applications of biopolymers for drugs and probiotics delivery. *Polymers*, **2021**, *13*(16), 1–32.
36. Mariana, M., Alfatah, T., Abdul Khalil, H.P.S., Yahya, E.B., Olaiya, N.G., Nuryawan, A., Mistar, E.M., Abdullah, C.K., Abdulmadjid, S.N., Ismail, H. A current advancement on the role of lignin as sustainable reinforcement material in biopolymeric blends. *J. Mater. Res. Technol.*, **2021**, *15*, 2287–2316.
37. Habibi, H., Khosravi, K. Effective variables on production and structure of xanthan gum and its food applications: a review. *Biocat. Agri. Biotechnol.*, **2017**, *10*(4), 130–140.
38. Mota, G., Pereira, R. A comparison of the rheological behavior of xanthan gum and diutan gum aqueous solutions. *J. Braz. Soc. Mech. Sci. Eng.*, **2022**, *44*, 117.
39. Lopes, B., Lopes, L., Vinícius. et. al. Xanthan gum: properties, production conditions, quality and economic perspective. *J. Food. Nutri. Res.*, **2015**, *54*, 185–194.
40. Patel, J., Maji, B., Moorthy, H.N., Maiti, N.S. Xanthan gum derivatives: review of synthesis, properties and diverse applications. *RSC Adv.*, **2020**, *10*, 27103–27136.

41. Joseph, S.M., Krishnamoorthy, S., Paranthaman, R., Moses, J.A., Andharamakrishnan, C. A review on source-specific chemistry, functionality, and applications of chitin and chitosan. *Carbohydr. Polym. Technol. Appl.*, **2022**, *2*, 1–15.
42. Guarino, V., Caputo, T., Altobelli, R., Ambrosio, L. Degradation properties and metabolic activity of alginate and chitosan polyelectrolytes for drug delivery and tissue engineering applications. *AIMS Mater. Sci.*, **2015**, *2*, 497–502.
43. Basa, S., Nampally, M., Honorato, T., Das, S.N., Podile, A.R., Gueddari, N.E. El., Moerschbacher, B.M. The pattern of acetylation defines the priming activity of chitosan tetramers. *J. Am. Chem. Soc.*, **2020**, *142*, 1975–1986.
44. Janani, G., Kumar, M., Chouhan, D., Moses, J.C., Gangrade, A., Bhattacharjee, S., Mandal, B.B. Insight into silk-based biomaterials: from physicochemical attributes to recent biomedical applications. *ACS Appl. Bio. Mater.*, **2019**, *2*(12), 5460–5491.
45. Bandyopadhyay, A., Chowdhury, S.K., Dey, S. et al. Silk: a promising biomaterial opening new vistas towards affordable healthcare solutions. *J. Indian. Inst. Sci.*, **2019**, *99*, 445–487.
46. Khoo, C.S., Knorr, D. Grand challenges in nutrition and food science technology. *Front. Nutr.*, **2014**, *1*(4), 1–3.
47. Gupta, I., Cherwoo, L., Bhatia, R., Setia, S. Biopolymers: implications and application in the food industry. *Biocatal. Agric. Biotechnol.*, **2022**, *46*, 102534.
48. Chausali, N., Saxena, J., Prasad, R. Recent trends in nanotechnology applications of bio-based packaging. *J. Agri. Food. Res.*, **2022**, *7*, 1–24.
49. Balart, R., Montanes, N., Dominici, F., Boronat, T., Torres-Giner, S. Environmentally friendly polymers and polymer composites. *Materials (Basel)*, **2020**, *13*(21), 1–6.
50. Yaradoddi, J.S., Banapurmath, N.R., Ganachari, S.V., Soudagar, M.E.M., Mubarak, N.M., Hallad, S., Hugar, S., Fayaz, H. Biodegradable carboxymethyl cellulose based material for sustainable packaging application. *Sci. Rep.*, **2020**, *10*(1), 21960.
51. Priyadarshi, R., Kim, H-Ji., Rim, J.W. Effect of sulfur nanoparticles on properties of alginate-based films for active food packaging applications. *Food. Hydrocoll.*, **2020**, *110*, 106155.
52. Costa, S.M., Ferreira, D.P., Teixeira, P., Ballesteros, L.F., Teixeira, J.A., Fangueiro, R. Active natural- based films for food packaging applications: the combined effect of chitosan and nanocellulose. *Int. J. Biol. Macromol.*, **2021**, *30*(177), 241–251.
53. Slosarczyk, A., Klapiszewska, I., Jędrzejczak, P., Klapiszewski, Ł., Jesionowski, T. Biopolymer- based hybrids as effective admixtures for cement composites. *Polymers*, **2020**, *12*(1180), 1–15.
54. Magalhaes, S., Alves, L., Medronho, B., Fonseca, A.C., Romano, A., Coelho, J.F.J., Norgren, M. Brief overview on bio-based adhesives and sealants. *Polymers*, **2019**, *11*(1685), 1–20.
55. Tourtelot, J., Bourges, A., Keita, E. Influence of biopolymers on the mechanical behavior of earth- based building materials. *Recent. Prog. Mater.*, **2021**, *3*(3), 1–17.
56. Soldo, A., Miletic, M., Auad, M.L. Biopolymers as a sustainable solution for the enhancement of soil mechanical properties. *Sci. Rep.*, **2020**, *10*(267), 1–13.
57. Mariappan, N. Recent trends in nanotechnology applications in surgical specialties and orthopedic surgery. *Biomed. Pharmacol. J.*, **2019**, *12*(3), 1095–1127.
58. Murugesan, S., Scheibel, T. Chitosan-based nanocomposites for medical applications. *J. Polym. Sci.*, **2021**, *59*, 1603–1739.

59. Messmer, E.M. The pathophysiology, diagnosis, and treatment of dry eye disease. *Deutsc. Arztebl. Int.*, **2015**, *112*, 71–81.
60. Elda M., M.-M., Torres Castillo Nora, E., Rodrigo, M.-G., Sofia Liliana, L.-S., Roberto, P.-S., Juan Eduardo, S.-H. Modern world applications for nano-biomaterials: tissue engineering and COVID-19. *Front. Bioeng. Biotechnol.*, **2021**, *9*, 1–16.
61. Pimentel, C.R., Ko, S.K., Caviglia, C., Wolff, A., Emneus, J., Keller, S.S., Dufva, M. Three-dimensional fabrication of thick and densely populated soft constructs with complex and actively perfused channel network. *Acta. Biomater.*, **2018**, *65*, 174–184.
62. Montoya, C., Du, Y., Gianforcaro, A.L. et al. On the road to smart biomaterials for bone research: definitions, concepts, advances, and outlook. *Bone. Res.*, **2021**, *9*(12), 1–16.
63. Patel, N., Feofilovs, M., Blumberga, D. Agro biopolymer: a sustainable future of agriculture – state of art review. *Environ. Climate. Technol.*, **2022**, *26*(1), 499–511.
64. Merino, D., Salcedo, M.F., Mansilla, Y., Casalounge, C.A., Alvarez, V.A. Development of sprayable sodium alginate-seaweed agricultural mulches with nutritional benefits for substrates and plants. *Waste Biomass Valor.*, **2021**, *12*(54).
65. Parente, J.F., Sousa, V.I., Marques, J.F., Forte, M.A., Tavares, C.J. Biodegradable polymers for microencapsulation systems. *Adv. Polym. Technol.*, **2022**, *2022*, 1–43.
66. Wilson, H.T., Xu, K., Taylor, A.G. Transcriptome analysis of gelatin seed treatment as a biostimulant of cucumber plant growth. *Sci. World. J.*, **2015**, *391234*, 1–14.
67. Lopez Velazquez, JC., Rodríguez, R., Espinosa, H., Andrews, H. Gelatin–chitosan–PVA hydrogels and their application in agriculture. *J. Chem. Technol. Biotechnol.*, **2019**, *94*(11), 3495–3504.
68. Effiong, D.E., Uwah, T.O., Jumbo, E.U., Akpabio, A.E. Nanotechnology in cosmetics: basics, current trends and safety concerns—a review. *Adv. Nanopart.*, **2020**, *09*(01), 1–22.
69. Sionkowska, A., Musiał, K., Gadomska, M., Adamiak, K. Fish collagen and chitosan mixtures as a promising biomaterial for potential use in medicine and cosmetic industry. *Eng. Biomater.*, **2022**, *164*, 16–24.
70. Higgs, J. How to meet military packaging standards & specifications. 2020.
71. Nayak, R., Wang, L., Padhye, R. *Electronic textiles: smart fabrics and wearable technology*. Elsevier Ltd, 2015, pp. 239–256.
72. Nechyporchuk, O., Yu, J., Nierstrasz, V.A., Bordes, R. Cellulose nanofibril-based coatings of woven cotton fabrics for improved inkjet printing with a potential in e-textile manufacturing. *ACS Sustain. Chem. Eng.*, **2017**, *5*, 4793.

CHAPTER 10

REVIEW ON DYE-SENSITIZED SOLAR CELLS (DSSCS): SMART MATERIAL FOR RENEWABLE ENERGY

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ABSTRACT

Dye-sensitized solar cell proposed by M. Gratzel in 1991 was based on a ruthenium complex with 11% efficiency. Now, DSSC has achieved above 14% efficiency with various other novel photosensitizers and other designed metal–organic complexes. DSSC offers an efficient and easy synthesis route that can be successfully implemented for future energy supply. It can be best utilized for low-powered devices at ambient conditions. DSSCs have been reported to perform better under ambient light conditions, therefore many researchers are trying to obtain the optimized dye-based solar cell which could become an alternative to the existing inorganic solar cells. Molecular engineering and *in silico* investigations (by utilizing "Density functional theory and time-dependent density functional theory") have resulted in many novel photosensitizers. Therefore, as a smart renewable energy material DSSC has been chosen for discussion in this chapter. This chapter discusses the molecular architecture and effect of double donor and acceptor moieties on the performance of dye-based solar cell.

10.1 INTRODUCTION

Due to the environmental friendly nature and of easy synthesis techniques, dye-based solar cells are now trending research area in the organic photovoltaics. First DSSC was proposed by Gratzel's group using ruthenium (Ru) complex as a photosensitizer [1–4]. An interesting thing about DSSC is that these can perform better than inorganic solar cells in the ambient light conditions [5]. Since 1991, DSSC has improved a lot in terms of efficiency, and the progress on the metal free organic dyes is significant. The mechanism of charge transport is shown in Figure 10.1. Significant improvement on the efficiency has been obtained in the last decade [6]. Some of the important reported results which showed improved efficiency are developed by Nazeeruddin et al., with efficiency of 11.18% [7], Chen et al., with efficiency of 11.50% [8], and Wang et al., reported 11.16% [9]. Mathew et al., reported 13% [10], further we have seen that the group of Kakiage et al. reported efficiency of the cell more than 14% [2]. The efficiency chart of DSSC is shown in Figure 10.2. The widely utilized strategy of designing novel molecular structure is based on the donor-bridge-acceptor (D-π-A) model [11]. An increase in the absorption wavelength of the dye is generally achieved by improving the electron-donating strength of donor molecules or by expanding the bridging unit or it could be done by enhancing the acceptor site. D-π-A molecular design has led to the development of unique structures such as double donor-π bridge-acceptor or double acceptor structures and various other molecular structures are also engineered [12, 13].

The charge transport mechanism part of the DSSC is illustrated in Figure 10.1, that include three main steps where the first step is to absorb the photon energy to excite the dye electron, the second part is to transfer this electron to the semiconducting material (generally taken TiO_2 as reference material for photoanode) and then in final step it is to regenerate the oxidized dye through electrolyte [15]. Dye molecule excites the electron to its LUMO level, as the electron reaches the excited level it transfers to the semiconductor material which lies at a lower level than the dye's LUMO level. From there the charge is extracted toward the photoelectrode and this charge then supplied back through the counter electrode utilizing the electrolyte as mediator.

For better performance of the device, the designed sensitizer should have certain characteristics which include its wide absorption region from visible to near infrared, chemical stability of the dye molecule and the frontier molecular energy orbitals should be aligned with the semiconducting material's energy levels, and with electrolyte utilized in the cell [16].

The best-known DSSCs are based on mainly ruthenium dye complexes and porphyrins metal complexes [17, 18]. The disadvantage with metal-organic dyes is their high cost of synthesis route and their toxicity is also not good for the environment. Therefore, organic dyes which do not include metal element are the interest of the researchers to look for efficient DSSC. Some of the photosensitizers that are widely utilized for preparing metal-free organic dyes are coumarin, diphenylamine, triphenylamine, indoline, phenothiazine, naphthalene, and many more other organic molecules [19]. The advantage of these materials is that they can tuned according to the desire of the devices.

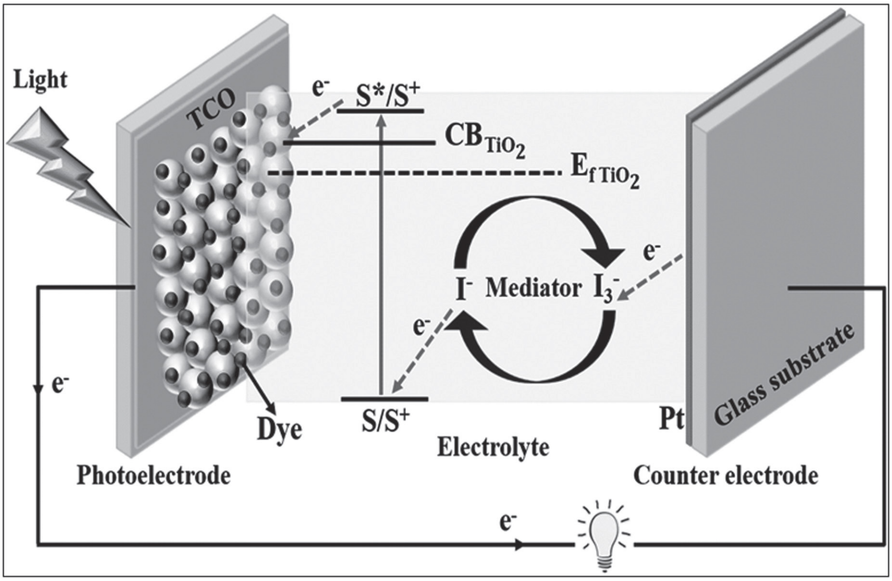


FIGURE 10.1 Working of the DSSC [14]. ⏎

Source: Reprinted from Ref. [14]. https://creativecommons.org/licenses/by/4.0/

Further in Figure 10.2, the progress of the best cell efficiencies (taken from the NREL website) is graphically represented where dye-based solar cells have achieved more than 14% efficiency since its beginning which opens the path for researchers to work on the improvement of its efficiency so that it could reach around 20% or more as achieved by the other inorganic material based solar cells.

To improve the performance of the DSSC, we may choose to alter donor moiety or we may choose to play with acceptor moiety so that new molecular energy orbitals which are formed due to the donor–acceptor interaction, are aligned with the semiconducting material's energy levels. We have seen from the past published papers that to improve the efficiency of the cell, more than one donor is the appropriate choice in designing the dye complex [12]. Some papers have reported that increasing the acceptor unit in the donor–acceptor template also helps in improving the V_{oc} and short J_{sc} which ultimately increases the efficiency of the designed cell [20]. Lowering of the LUMO energy levels improves the charge transfer rate and it stops the recombination of charges. Therefore, acceptor moieties become important in designing the photosensitizers because LUMO mostly gets contribution from the acceptor moiety (Table 10.1).

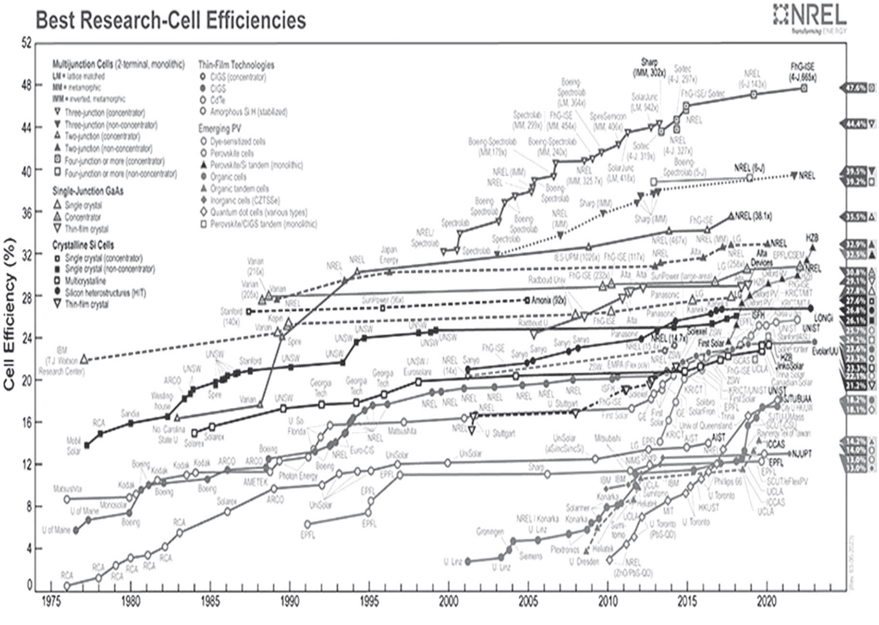


FIGURE 10.2 Efficiency chart of solar cells. ⏎

Source: https://www.nrel.gov/pv/cell-efficiency.html

Here, in this chapter, which is taken from our published papers [21, 22], we have chosen 10 dyes for review where dyes from 1 to 8 are based on "coumarin and triphenylamine as electron donor sites which are bridged with four different electron acceptor units like barbituric acid (Ba), cyanoacetic acid (Cy), hydantoin (Hy), and rhodamine-*n*-acetic acid (Rh), via thiophene molecule." Therefore, the first four dyes are based on donor-π-acceptor model that is "C-π-Ba, C-π-Cy, C-π-Hy, and C-π-Rh." Then other four are based on double donor-π-acceptor model, that is, "T-C-π-Ba, T-C-π-Cy, T-C-π-Hy, and T-C-π-Rh." Further two more dyes that is dye 9 and dye 10 have been reviewed and found to have absorption in the near-infrared region of the visible spectrum. Here, "carbazole" is donor and acceptor units are "naphthalimide and benzothiadiazole" moieties. Dye 9 "C-π-NI" is designed on the model of (donor-πbridge-acceptor) and Dye 10 "C-π-NI-BT" is designed on the model of (donor-πbridge-double acceptor) [22]. All dye structures from dyes 1 to 10 are shown in Figure 10.3.

TABLE 10.1 Some of the Commonly Used Donors, Acceptors, and Bridging Molecules are Shown Below ⏎

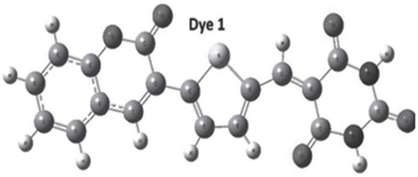
Donors	Acceptors	Bridge Molecules
1. Anthracene	1. Fullerene	1. Thiophene
2. Phenanthrene	2. Pyridine	2. Pyrrole
3. Coronene	3. Pyrimidine	3. Furan
4. Naphthalene	4. Acetic acid	4. Benzene
5. Diphenylamine	5. Butanoic acid	5. Ethylene
6. Triphenylamine	6. Pyrazine	6. Norbornadiene
7. Carbazole	7. Cyanoacetic acid	7. Sesquinorbornatriene
8. Indene	8. Rhodanine acid	
9. Iso-Indene	9. Naphthalimide	
10. Benzene	10. TCNQ	

10.2 COMPUTATIONAL DETAILS

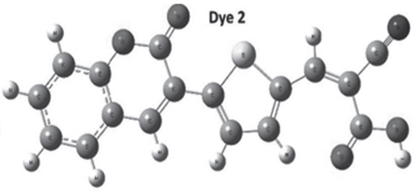
Dyes from 1 to 8 are based on donor-πbridge-acceptor and double donor-πbridge-acceptor models which are designed using the Gaussview [23] interface. The electronic structure calculations are performed utilizing the software that is Gaussian 09 [24]. Theoretical calculations are performed at "B3LYP functional along with the 6-31G(d,p)" basis set under the framework of density functional theory. Further to compute the excited state, "CAM-B3LYP functional [25] along with the 6-311++G(d,p)" basis set was employed.

In addition, further for dyes 9 and 10 where donor-πbridge-acceptor and donor-πbridge-double acceptor respective model was used, the calculations were done on Gaussian16W [26] software package. The functional "B3LYP and basis set cc-pVDZ" were used in these calculations. The excited state properties are calculated at "CAM-B3LYP" and the same basis set.

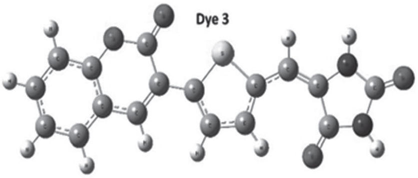
Optimized dyes from 1 to 10 are shown in Figure 10.3.



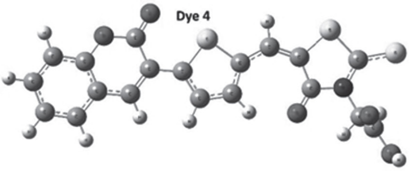
D1. "C-π-Ba"



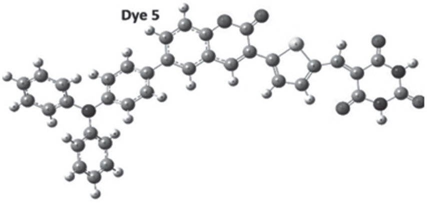
D2. "C-π-Cy"



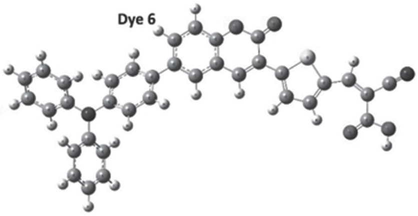
D3. "C-π-Hy"



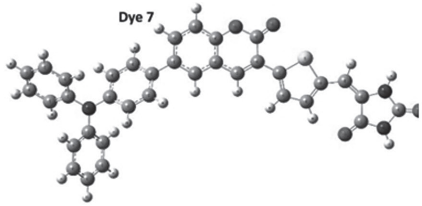
D4. "C-π-Rh"



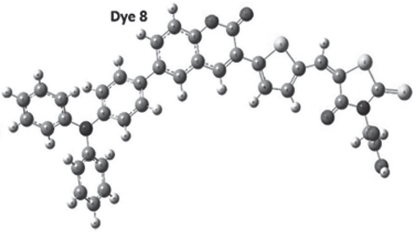
D5. "T-C-π-Rh"



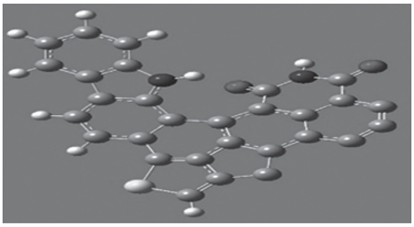
D6. "T-C-π-Cy"



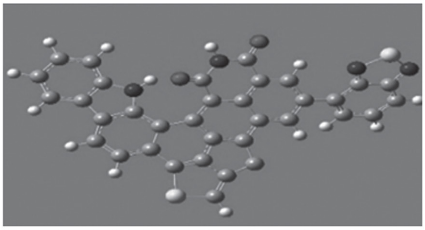
D7. "T-C-π-Hy"



D8. "T-C-π-Rh"



D9. "C-π-NI"



D10. "C-π-NI-BT"

FIGURE 10.3 Optimized geometries of D1 to D10 dyes. ⏎

The optoelectronic performance parameters for dyes are calculated utilizing the following formulae [27].

The efficiency of DSSC is given as

$$\eta = \frac{V_{oc}\ J_{sc}\ FF}{Is} * 100\% \tag{10.1}$$

Factors influencing effficiency is determined by the following equation:

$$J_{sc} = \int LHE(\lambda)\phi_{inject} * \eta_{collect}\, d\lambda \tag{10.2}$$

The absorption is also one of the important factors in determining the short-circuit photocurrent density therefore the red-shifted dyes would show the better performance as compared to the blue-shifted dyes. Thus, the LHE and ϕ_{inject} play the key role in the control of the J_{sc}. The other way to improve the Jsc is the improvement in the ΔG^{inject} values. The larger the values of the ΔG^{inject} the better charge injection efficiency ϕ_{inject} will be there [28]:

$$\Delta G^{\text{inject}} = E_{\text{ox}}^{\text{dye*}} - E_{\text{CB}}^{\text{TiO}_2} \tag{10.3}$$

$\text{E}_{\text{CB}}^{\text{TiO}_2}$ redox potential of the C.B. of the $\text{TiO}_2 = -4.0$ eV [29].

$$E_{\text{ox}}^{\text{dye*}} = E_{\text{ox}}^{\text{dye}} - \lambda_{\text{max}}^{\text{ICT}} = -E_{\text{HOMO}} - \lambda_{\text{max}}^{\text{ICT}} \tag{10.4}$$

$E_{\text{ox}}^{\text{dye}}$ from the Koopman's theorem is equal to the (-HOMO) energy. Also $\lambda_{\text{max}}^{\text{ICT}}$ is the energy corresponding to the intramolecular charge transfer.

Regeneration driving force (ΔG_{reg}). This can be approximated as

$$(\Delta G_{reg}) = (E_{ox}^{\text{dye}} - 4.8 \text{ eV}) \text{ or } (-E_{\text{HOMO}}^{\text{DYE}} - 4.8) \text{ eV} \tag{10.5}$$

where −4.8 eV is the iodide electrolyte's redox potential [21].

The V_{OC} is an experimentally determined parameter. Due to the various previous studies on the DSSCs have shown that there is some analytical relationship exists between V_{oc} and LUMO energy levels of the dye that is shown as

$$V_{\text{oc}} = -E_{\text{LUMO}}^{\text{dye}} - \text{C.B.}\ (E_{\text{TiO}_2}) \tag{10.6}$$

where C.B. is the semiconductor's conduction-band edge.

10.3 RESULTS AND DISCUSSION

We have focused on the electronic and optical parameters to describe the behavior of double donor moieties from dyes 1 to 8, and double acceptor moieties' impact on the performance of DSSC for dye 9 and dye 10 (Figure 10.4).

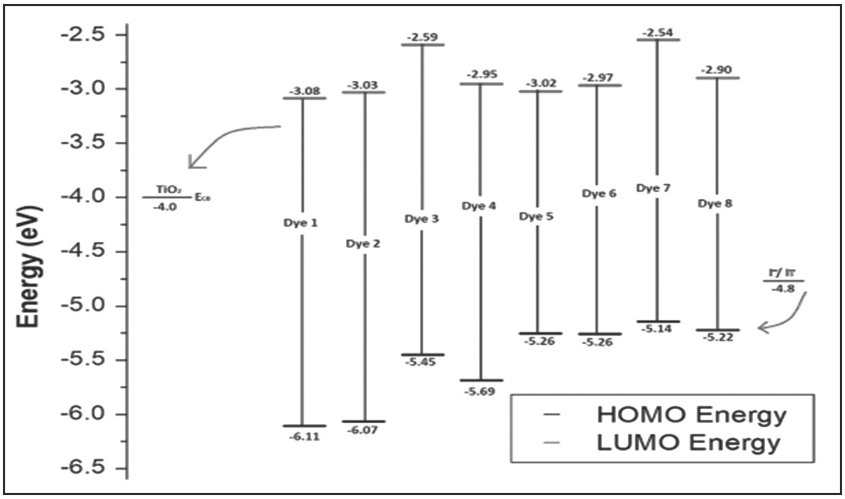


FIGURE 10.4 Energy diagram of dyes 1 to 8, electrolyte is iodide solution, TiO_2 is photoanode. ⏎

10.3.1 IMPACT OF DOUBLE-DONOR UNITS ON THE PERFORMANCE OF DSSC: DYES 1 TO DYES 8 ARE DISCUSSED BELOW

10.3.1.1 DYES HAVING BARBITURIC ACID ACCEPTOR UNIT

We have two dyes where barbituric acid is used as acceptor unit which are dye 1 and dye 5. The absorption wavelength of the dye 1 is at 437 nm and for dye 5 the absorption wavelength is at 445 nm. The oscillator strength for dye 1 is at 1.306 and for dye 5 it is 1.516, while the LHE value for dye 1 is 0.951 eV and for dye 5 it is 0.969 eV (reported in Table 10.2). The other photovoltaic parameters suggest that charge injection free energy for dye 1 and dye 5 is −0.730 eV and −1.530 eV, respectively. From the calculated parameters it is clearly noticed that dye with double-donor moiety shows improved photovoltaic characteristics as compared to the single-donor moiety. Therefore, it is suggested that the double-donor approach is superior for photovoltaic usage in alteration to the single-donor approach.

10.3.1.2 DYES HAVING CYANOACETIC ACID (CY) ACCEPTOR UNIT

Similarly, dye 2 and dye 6 have cyanoacetic acid as the acceptor unit in both dyes. The dye 6 has an additional donor triphenylamine which is added along with the first donor coumarin to see the effect on the performance of the designed DSSC. Here the reported absorption wavelength for dye 2 is 431 nm and for dye 6 it is 438 nm (reported in Table 10.2), this suggests that absorption wavelength increases as we move from single donor approach to the double donor approach in designing the photosensitizer. Further, the other photovoltaic parameters like oscillator strength, charge injection energy, and light harvesting efficiency all significantly suggests an improvement in the values of dye 6 as compared to the dye 2. Hence, we can infer from our reviewed dye molecule that the double-donor approach is superior as compared to the single-donor approach.

TABLE 10.2 For Dyes 1 to 8, *Max abs* Wavelength is Shown in nm, Oscillator Strength, and Light Harvesting Efficiency is in eV [21] ⏎

Photosensitizers	λ_{max} (nm)	F	LHE (eV)
Dye 1	437.00	1.306	0.951
Dye 2	431.00	1.174	0.933
Dye 3	460.00	1.081	0.917
Dye 4	487.00	1.314	0.951
Dye 5	445.00	1.516	0.969
Dye 6	438.00	1.523	0.970
Dye 7	463.00	1.382	0.958
Dye 8	490.00	1.611	0.975

10.3.1.3 DYES HAVING HYDANTOIN (HY) ACCEPTOR UNIT

For dye 3 and dye 7 the hydantoin acid is the acceptor unit in both dyes. While the dye 7 is having the double donor system as triphenylamine is added with coumarin here. Therefore, the photovoltaic performance is compared for dye 3 and dye 7 which represent single-donor and double-donor systems. The absorption wavelength for dye 3 is at 460 nm and for dye 7 it is at 463 nm. This suggests that there is a slight improvement in the designed dye where the double donor approach is found to be superior as compared to the single donor approach. Further the other photovoltaic parameters reported in Tables 10.2 and 10.3 suggests that improvements are reported in dye 7 as compared to the dye 3. Therefore, we suggest that dyes with a double-donor approach prove to be the better approach for designing the photosensitizer as compared to the single-donor approach.

TABLE 10.3 For Dyes 1 to 8, Computed ΔG^{inject}, E_{OX}^{dye*}, E_{OX}^{dye}, and λ_{max}^{ICT} in (eV) [21] ⏎

Photosensitizers	ΔG^{inject} (eV)	E_{OX}^{dye*} (eV)	E_{OX}^{dye} (eV)	λ_{max}^{ICT} (eV)	V_{oc} (eV)
Dye 1	–0.730	3.270	6.110	2.840	0.9160
Dye 2	–0.800	3.200	6.070	2.870	0.9690
Dye 3	–1.240	2.760	5.450	2.690	1.4100
Dye 4	–0.850	3.150	5.690	2.540	1.0470
Dye 5	–1.530	2.470	5.260	2.790	0.9790
Dye 6	–1.570	2.430	5.260	2.830	1.0340
Dye 7	–1.540	2.460	5.140	2.680	1.4560
Dye 8	–1.310	2.690	5.220	2.530	1.1020

10.3.1.4 DYES HAVING RHODANINE-N-ACETIC ACID (RH) ACCEPTOR UNIT

The dye 4 and dye 8 both have the same acceptor unit in the form of rhodamine-n-acetic acid. And dye 8 has two donors while dye 4 has only one donor as coumarin. The absorption wavelength for dye 4 is at 487 nm and for dye 8 it is 490 nm. The oscillators strength for dye 4 and dye 8 are 1.314 and 1.611, respectively. The open-circuit voltage for dye 4 and dye 8 are 1.047 eV and 1.102 eV, respectively (see Table 10.3). The other photovoltaic parameters like LHE and charge injection free energy also suggest that dye 8 with double donor system have improved performance as compared to the single donor system of dye 4. Hence, we infer from our analysis that double-donor system is superior as compared to the single-donor system in designing the photosensitizer.

10.3.2 EFFECT OF DOUBLE ACCEPTOR GROUPS ON THE PERFORMANCE OF DSSC: DYE 9 AND DYE 10 ARE DISCUSSED BELOW

To design the higher wavelength absorption dyes, the frontier molecular energy orbitals play an important role. The LUMO levels of the designed dyes should be close to the semiconductor's fermi energy level so that efficient charge transfer could take place from the LUMO of the photosensitizer. Therefore, here we have reviewed the effect of double acceptor units on the performance of the photosensitizers by taking two sets of designed molecules. The two sets of molecules where the absorption is found in the near infrared region are based on double acceptor approach. These are denoted as dye 9 and dye 10 as shown in Figure 10.3. The dye 9 is "carbazole-thiophene-naphthalimide" and dye 10 is "carbazole-thiophene-naphthalimide-benzothiadiazole." Here, we have chosen In_2O_3 as the reference anode because of its suitable HOMO and LUMO levels as compared with the photosensitizers and HLG energy of In_2O_3 (is 3.5 eV) [30]. Further, we have discussed various other parameters of dye 9 and dye 10.

10.3.2.1 DYES 9 AND 10, PHOTOVOLTAIC PERFORMANCE ANALYSIS

From Tables 10.4 and 10.5, the dye 9 shows λ_{max} at 1432 nm, and dye 10 shows λ_{max} at 1351 nm. The high absorption wavelength is probably because of their better alignment of the LUMO levels with the conduction band edge of the semiconducting material In_2O_3 [31]. Further, the designed dyes have taken naphthalimide and benzothiadiazole as the acceptor units which are reported to be strong electron acceptor units. Therefore, choosing a strong acceptor unit is also one of the important parameters for designing the photosensitizer. The double acceptor unit here shows better ΔG_{inject} values as compared to the single acceptor unit where the dye 10 has more negative value as compared to the dye 9. This suggests the charge injection will be faster in the double acceptor photosensitizer as compared to the single acceptor unit. From the open-circuit voltage V_{OC} calculation we found that dye 9 and dye 10 have reported values to be 1.36 eV and 1.49 eV, respectively, which suggests that double-acceptor approach proves to be better as compared to the single acceptor approach in designing the photosensitizer.

TABLE 10.4 For Dyes 9 and 10, HOMO, LUMO, HLG Energy, Max abs Wavelength (in nm), and Oscillator Strength *F*, LHE (in eV) is Calculated ⏎

Photosensitizer	HOMO (eV)	LUMO (eV)	HLG (eV)	λ_{max} (nm)	F	LHE (eV)
Dye 9 (C-π-NI)	–5.76	–4.04	1.72	1432	0.0008	0.002
Dye 10 (C-π-NI-BT)	–5.66	–3.91	1.75	1351	0.0009	0.003

TABLE 10.5 For Dyes 9 and 10, Computed "ΔG^{inject}, E_{OX}^{dye*}, E_{OX}^{dye}, and λ_{max}^{ICT} in (eV), ΔG_{reg} (eV), eV_{OC} (in eV) Energy" ⏎

Photosensitizer	ΔG^{inject} (eV)	E_{OX}^{dye*} (eV)	E_{OX}^{dye} (eV)	λ_{max}^{ICT} (eV)	ΔG_{reg} (eV)	V_{OC} (eV)
Dye 9 (C-π-NI)	–0.5	4.9	5.766	0.866	0.96	1.36
Dye 10 (C-π-NI-BT)	–0.651	4.749	5.667	0.918	0.86	1.49

10.4 CONCLUSION

From this reviewed chapter on the DSSC as the smart material for renewable energy, we have chosen 10 photosensitizers where the effect of double donor units and the effect of double acceptor units on the performance of DSSC was discussed majorly. From the above analysis of dyes 1 to 8, it was clearly inferred from the obtained results that the absorption wavelength of the double donor dyes is higher as compared to the single donor dyes. Further, the other important parameters like charge injection driving force, light harvesting efficiency, and V_{oc}, J_{sc} have been improved for double donor photosensitizers because of the extended conjugation length which favors the easy charge transfer toward the acceptor unit. Therefore, these modeled dye sensitizers suggest us increasing the donor moieties can increase the performance of the DSSC. And from the two more dyes where effect of a double-acceptor unit was reviewed, that is, dye 9 and dye 10, we found that double double-acceptor unit shows better photovoltaic parameters as compared to the single acceptor unit based photosensitizers. Therefore, it is one of the interesting findings in designing the efficient photosensitizers that double acceptor site as well as double donor site could show better photovoltaic characteristics as compared to the single donor and acceptor based photosensitizers. Therefore, we are of strong opinion that this study in the form of reviewed DSSC material could also be useful for experimentalists to design efficient photosensitizers.

10.5 FUTURE SCOPE AND LIMITATIONS

As a renewable energy material reviewed dyes or photosensitizers for DSSC is the perfect choice to work under ambient light conditions where efficiency is not very much of concern. The portable electronic gadgets can utilize the power output from these devices. Further, the scope of its application is wider due to the presence of low-powered electronic devices like small sensors, mobile phones etc. where DSSC could provide an alternative to the silicon-based solar cells.

On the limitation aspect, DSSC faces a challenge of novel materials where efficiency could reach upto 20% to 25% as inorganic material like silicon-based solar cells have reached. Further, the challenge of its dye life is of concern because the electrolyte which is used for smooth functioning of DSSC faces the challenge of deterioration in atmospheric conditions.

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KEYWORDS

- **DSSC**
- **donor**
- **acceptor**
- **DFT**
- **TDDFT**
- **photosensitizers**

REFERENCES

1. Brian O’ Regan, M.G. A low-cost, high efficiency solar cell based on dye-sensitized colloidal TiO_2 films. *Nature*, **1991**, *354*, 56–58.
2. Kakiage, K., Aoyama, Y., Yano, T., Oya, K., Fujisawa, J.I., Hanaya, M. Highly-efficient dye-sensitized solar cells with collaborative sensitization by silyl-anchor and carboxy-anchor dyes. *Chem. Commun.*, **2015**, *51*(88), 15894–15897, https://doi.org/10.1039/c5cc06759f.
3. Wan, Z.Q., Zhou, L.L., Jia, C.Y., Yao, X.J., Shi, Y. Computational study on triphenylamine-based dyes containing benzimidazole units for dye-sensitized solar cells. *Adv. Mater. Res.*, **2013**, *668*, 110–114, https://doi.org/10.4028/www.scientific.net/AMR.668.110.
4. Selopal, G.S. et al. Metal-free organic dyes for TiO_2 and ZnO dye-sensitized solar cells. *Sci. Rep.*, **2016**, *6*(January), 1–12, https://doi.org/10.1038/srep18756.
5. Shalini, S., Balasundaraprabhu, R., Kumar, T.S., Prabavathy, N., Senthilarasu, S., Prasanna, S. Status and outlook of sensitizers/dyes used in dye sensitized solar cells (DSSC): a review. *Int. J. energy Res.*, **2016**, *40*, 1303–1320 https://doi.org/10.1002/er.3538
6. Gong, J., Sumathy, K., Qiao, Q., Zhou, Z. Review on dye-sensitized solar cells (DSSCs): advanced techniques and research trends. *Renew. Sustain. Energy Rev.*, **2017**, *68*(December 2015), 234–246, https://doi.org/10.1016/j.rser.2016.09.097.
7. Abate, A. et al. Energy & environmental science. *Energy Environ. Sci.*, **2015**, *8*, 2946–2953, https://doi.org/10.1039/C5EE02014J.
8. Chen, J. et al. Backbone conformation tuning of carboxylate-functionalized wide band gap polymers for efficient non-fullerene organic solar cells. *Macromolecules*, **2019**, *52*(1), 341–353, https://doi.org/10.1021/acs.macromol.8b02360.

9. Wang, H., Bao, B., Hu, X., Fang, J.K. Efficient small molecule organic dyes containing different bridges in donor moieties for dye-sensitized solar cells. *Electrochim. Acta*, **2017**, *250*, 278–284, https://doi.org/10.1016/j.electacta.2017.08.089.
10. Mathew, S. et al. Dye-sensitized solar cells with 13% efficiency achieved through the molecular engineering of porphyrin sensitizers. *Nat. Chem.*, **2014**, *6*(3), 242–247, https://doi.org/10.1038/nchem.1861.
11. Bourass, M. et al., DFT and TD-DFT calculation of new thienopyrazine-based small molecules for organic solar cells. *Chem. Cent. J.*, **2016**, *10*(1), 67, https://doi.org/10.1186/s13065-016-0216-6.
12. Jungsuttiwong, S., Tarsang, R., Sudyoadsuk, T., Promarak, V., Khongpracha, P., Namuangruk, S. Theoretical study on novel double donor-based dyes used in high efficient dye-sensitized solar cells: the application of TDDFT study to the electron injection process. *Org. Electron.*, **2013**, *14*(3), 711–722, https://doi.org/10.1016/j.orgel.2012.12.018.
13. ElKhattabi, S. et al. Theoretical investigation of electronic, optical and photovoltaic properties of alkylamine-based organic dyes as sensitizers for application in DSSCs. *J. Mater. Environ. Sci.*, **2018**, https://doi.org/10.26872/jmes.2018.9.3.93.
14. Kokkonen, M. et al. Advanced research trends in dye-sensitized solar cells. *J. Mater. Chem. A*, **2021**, *9*(17), 10527–10545, https://doi.org/10.1039/d1ta00690h.
15. Fahim, Z.M.E., Aicha, Y.A., Bouzzine, S.M., Bouachrine, M., Hamidi, M. Modulation on dye/TiO_2 bending energy and charge transfer to high performance triphenylamine based sensitizers in solar cells: a DFT study. In *2018 6th International Renewable and Sustainable Energy Conference (IRSEC)*, 2018, pp. 1–5, https://doi.org/10.1109/IRSEC.2018.8702924.
16. Sharma, G.D. et al. Stepwise co-sensitization as a useful tool for enhancement of power conversion efficiency of dye-sensitized solar cells: the case of an unsymmetrical porphyrin dyad and a metal-free organic dye. *Org. Electron.*, **2014**, *15*(7), 1324–1337, https://doi.org/10.1016/j.orgel.2014.03.033.
17. Nguyen, T.D., Wu, C.G. Non-classical design of high-efficiency sensitizers for dye-sensitized solar cells. *J. Chinese Chem. Soc.*, **2018**, *65*(5), 511–522, https://doi.org/10.1002/jccs.201700399.
18. Yella, A, Lee, H.-W., Tsao, H.N., Yi, C., Chandiran, A.K., Nazeeruddin, M.K., Diau, E.W.-G., Yeh, C.-Y., Zakeeruddin, S.M., Graetzel, M. Porphyrin-sensitized solar cells with yield shorter electron lifetimes when used in the DSC. This faster interfacial charge recombina-cobalt (II/III)-based redox electrolyte tion, when compared with iodide/triiodide-based redox electrolytes (12–18), lowe. *Science*, **2011**, *334*, 629–633.
19. Koyyada, G. et al. A new series of EDOT based co-sensitizers for enhanced efficiency of cocktail DSSC: a comparative study of two different anchoring groups. *Molecules*, **2019**, *24*(19), 3554, https://doi.org/10.3390/molecules24193554.
20. Zheng, L. et al. Novel D-A-π-A-type organic dyes containing a ladderlike dithienocyclopentacarbazole donor for effective dye-sensitized solar cells. *ACS Omega*, **2017**, *2*(10), 7048–7056, https://doi.org/10.1021/acsomega.7b01387.
21. Siddiqui, S.A. Molecular modeling and simulation for the design of dye sensitizers with mono- and di-substituted donor moieties. *J. Comput. Electron.*, **2022**, *21*(1), 52–60, https://doi.org/10.1007/s10825-021-01839-9.
22. Rasheed, T., Kargeti, A., Ahmad, S. Design of two novel dyes having maximum absorption in infrared region : a DFT investigation. *Mater. Today Proc.*, **2022**, *68*(7), 2715–2719https://doi.org/10.1016/j.matpr.2022.06.267.

23. 2016. GaussView, Version 6, Dennington, Roy; Keith, Todd A.; Millam, John M. Semichem Inc., Shawnee Mission, KS, GaussView 6. *Gaussian*., **2016**.
24. Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G.A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H.P., Izmaylov, A.F., Bloino, J., Zheng, G., Sonnenberg, J.L., Had, M. et al. *Gaussian 09, revision D.01*. Gaussian Inc.: Wallingford, 2013, https://doi.org/10.1017/CBO9781107415324.004.
25. Yanai, T., Tew, D.P., Handy, N.C. A new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP). *Chem. Phys. Lett.*, **2004**, *393*(1–3), 51–57, https://doi.org/10.1016/j.cplett.2004.06.011.
26. Frisch, M.J. et al. *Gaussian 16*. Gaussian, Inc.: Wallingford CT, 2016.
27. Divya, V.V., Suresh, C.H. Density functional theory study on the donating strength of donor systems in dye-sensitized solar cells. *New J. Chem.*, **2020**, *44*(17), 7200–7209, https://doi.org/10.1039/d0nj00723d.
28. Shahnaz Ahmed, D.J.K. Charge transport in isoindigo- dithiophenepyrrole based D-A type oligomers : a DFT / TD-DFT study for the fabrication of fullerene-free organic solar cells. *J. Chem. Phys.*, **2018**, *5648*(1993), https://doi.org/10.1063/1.5055306.
29. Irfan, A., Jin, R., Al-Sehemi, A.G., Asiri, A.M. Quantum chemical study of the donor-bridge-acceptor triphenylamine based sensitizers. *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.* **2013**, *110*, 60–66, https://doi.org/10.1016/j.saa.2013.02.045.
30. Wagner, M., Hofinger, J., Setvín, M., Boatner, L.A., Schmid, M., Diebold, U. Prototypical organic-oxide interface: intramolecular resolution of sexiphenyl on In2O3(111). *ACS Appl. Mater. Interfaces*, **2018**, *10*(16), 14175–14182, https://doi.org/10.1021/acsami.8b02177.
31. Wagner, M., Hofinger, J., Setvín, M., Boatner, L.A., Schmid, M., Diebold, U. Prototypical organic-oxide interface: intramolecular resolution of sexiphenyl on In2O3(111). *ACS Appl. Mater. Interfaces*, **2018**, *10*(16), 14175–14182, https://doi.org/10.1021/acsami.8b02177.

CHAPTER 11

USING LIME WATER IN THE MANUFACTURING OF FERROCHROME ASH-BASED GEOPOLYMER CONCRETE

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ABSTRACT

Few studies have indicated that the use of lime water instead of potable water during the mixing of concrete could influence the reaction mechanism and strength development in concrete. In this study, the use of lime water has been investigated in the manufacturing of geopolymer concrete made out of ferrochrome ash (FCA) and fly ash (FA). FCA, one of the by-products of ferroalloy industries, has been employed as the primary source material. FA is a secondary source material source to aid the binder mix with adequate aluminum and silicon content. A blend of sodium hydroxide (NaOH) and sodium silicate (Na_2SiO_3) was adopted as an alkaline activator to foster the alkali-activation/geopolymerization reaction. Saturated lime water was used

instead of potable water during the concrete mixing process. The workability and compressive strength properties were investigated. The results demonstrate that additional lime source in the form of lime water during mixing offers a negative effect with respect to the compressive strength development of FCA–FA-based geopolymer concrete samples. The conclusions may motivate the researchers to improve the characteristics of FCA–FA-based geopolymer concrete further while encouraging to uptake a circular economy approach.

11.1 INTRODUCTION

The demand for cement production for making concrete has risen globally due to the overall development of civilization and the progress of society. According to a study [1], the consumption of concrete for every person on earth is approximately one cubic meter. Manufacturing of cement and its composites is accompanied by greenhouse gas emissions (CO_2, SO_x, NO_x), hence sustaining the ecological balance remains a top priority. Therefore, it is essential to go beyond the current knowledge and develop alternative binders that are sustainable and comparable to conventional cement regarding its properties. Geopolymer is a cement-less binder and is a promising field of research that not only utilizes industrial wastes at a large scale but also paves the route for synthesizing the new generation of low-carbon construction materials for wide commercial applications [2–4].

The aluminum and silicon oxides present in the source materials, such as FA and blast furnace slag (BFS)/ground granulated blast furnace slag (GGBFS), are activated by an alkaline solution consisting of a particular molar concentration of alkali hydroxides such as NaOH/KOH mixed with Na_2SiO_3 or K_2SiO_3 solutions at a fixed mass ratio. However, the rate of efflorescence has also been observed to increase systematically. Therefore, a sodium-based alkaline solution provides better strength development than potassium-based solutions. Following a complex reaction mechanism, the final product is a tetrahedral matrix unit involving aluminum and silicon, which is linked by oxygen and is formed depending upon the Al/Si ratio of the source materials used [5]. The primary objective for employing geopolymer concrete is attributable to its enhanced mechanical and durability aspects compared to typical cement-based concrete [6]. At the same time, the problem of increased CO_2 footprints along with the disposal of industrial wastes also gets alleviated. Figure 11.1 illustrates the constituents and advantages of geopolymer concrete in the present scenario.

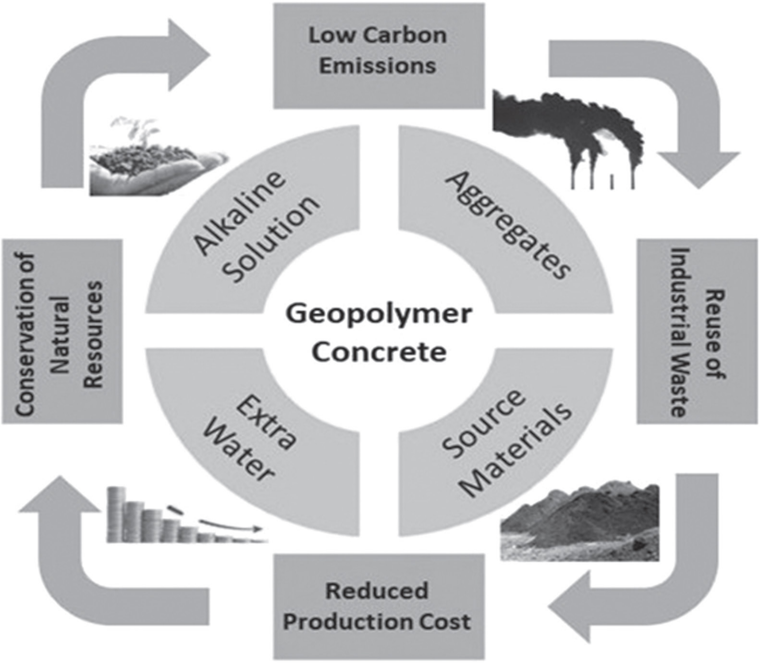
Low Carbon Emissions
Aggregates
Reuse of Industrial Waste
Source Materials
Reduced Production Cost
Extra Water
Conservation of Natural Resources
Alkaline Solution
Geopolymer Concrete

FIGURE 11.1 Constituents and advantages of geopolymer concrete. ⏎

Strength progression in geopolymer concrete is principally determined through the chemical framework of the source materials and alkaline solution, along with other considerations like curing temperature, fineness of materials, the concentration of alkali hydroxides, water-geopolymer solid ratio, moisture content of aggregates, and humidity conditions. The geopolymerization process involves the generation of sodium aluminate silicate hydrate (N-A-S-H), calcium aluminate silicate hydrate (C-A-S-H) type gels that expedite the strength progression and determine the setting process of the cast specimens [7, 8]. The structure of these gels could be modified or improved further by the addition of other silica-rich or calcium-rich minerals in the mix, and these gels could co-exist in the form of hybrid C-N-A-S-H gel that aids in the densification of the geopolymer matrix [9]. Source materials containing more calcium initiate C-A-S-H gels, while those with less or no calcium form N-A-S-H gels. However, the morphological characteristics are distinct from each other [10].

The building industry significantly contributes to global pollution levels, accounting for nearly 17% of the overall CO_2 emissions, with cement production single-handedly accounting for about 8%. Geopolymer composites have been estimated to decrease up to 80% of CO_2 emissions when judged against OPC-based composites [11]. This is because the geopolymer chemical reaction occurs at lower temperatures than the high-temperature kiln firing required for cement production. Additionally, geopolymer materials have a longer service life and better durability than traditional cement-based materials, reducing the need for frequent repairs and replacements. This reduces the overall carbon footprint associated with the production and transportation of construction materials. Furthermore, geopolymer-based insulation materials with excellent thermal properties can assist in reducing heating and cooling requirements in buildings, resulting in lower energy consumption and carbon emissions. However, these estimations cannot be generalized for geopolymers due to the variations in their production process. Thus, it can be stated that the fabrication of geopolymer composites emits comparatively less CO_2, and its wide implementation can certainly help mitigate carbon footprints and decrease environmental impacts [12].

Nearly 20–30 kg of ferrochrome ash (FCA) is produced as waste during each ton of ferrochrome product manufacturing. According to reports, global ferrochrome production has reached 6.5–9.5 million tonnes per year [13]. FCA has slag-like properties, which have proved to be advantageous as substitution of cement in concrete systems with improved strength and durable properties [13–16]. Meanwhile, India is one of the major ferrochrome manufacturers in the world, and its waste disposal is a serious environmental concern. Hence significant efforts are necessary to utilize FCA/FCS at a larger scale, preferably in the construction industry. Apart from cement-based composites, FCA/FCS could also be transformed into a potential raw material for pavements, ceramics, refractory materials, brick fabrication, hazardous hexavalent chromium remediation/treatment, and environmental-friendly composites such as geopolymers [17]. In terms of the reaction mechanisms, both FCA and slag can contribute to the formation of geopolymer gels by reacting with an alkaline activator. However, the presence of chromium oxide can affect the geopolymerization process and the final behavior of geopolymer material. According to the literature, FCA contains oxides of aluminum, silicon, magnesium, and iron, making it a feasible material for use as a source material for geopolymerization [18–21].

FA is an efficient precursor material that contains an adequate amount of aluminum and silicon oxides required for geopolymerization; hence, the geopolymer samples made with FA exhibit outstanding mechanical and durable properties [22, 23]. However, FA-incorporated geopolymer samples depend on the high-temperature curing conditions for their strength development. On the contrary, the reaction process is prolonged when cured under ambient conditions, leading to lower strength gain [20, 21], which limits the use of FA. Therefore, to improve its reactivity under ambient conditions, several researchers have recommended the addition of calcium-based materials in the geopolymer mixes [24, 25].

Besides, the utilization of lime as a calcium-based additive in geopolymer concrete manufacturing has proved to be beneficial in earlier investigations [26]. The inclusion of calcium into the mix helps in the reduction of setting times of the samples while simultaneously influencing the strength characteristics in the absence of heat curing [27]. This is because the additional calcium forms calcium-rich aluminosilicate gels, thus enhancing the end properties [28]. Furthermore, the existence of calcium hastens the dissolution rate of aluminum and silicon and significantly aids in the polymerization process. All of these reasons draw our interest to the significance of incorporating lime sources in the geopolymer mixes. Therefore, another method of boosting the calcium amount and the alkalinity has been adopted in this study, that is, through the utilization of saturated lime water instead of traditional tap water during the mixing process. A limited number of studies have been reported so far that utilize lime water during mixing to prepare cement-based concrete [29–31] with enhanced strength properties. However, no research has been found on its utility in the manufacturing of geopolymer concrete.

The study examines the effect of lime water in the mixing process. It is hypothesized that the inclusion of lime water would influence the strength development of the FCA–FA-based geopolymer mixes. Besides, a brief literature analysis on the development of geopolymer binders using ferrochrome wastes has been presented in Table 11.1 to comprehend the scope of the research progress. Few studies have been performed so far blending FA with FCA [32–35, 41, 45, 47]. Therefore, the current research simultaneously intends to further the understanding of ambient cured FCA–FA-based geopolymer concrete.

11.2 MATERIALS AND METHODS

11.2.1 MATERIALS

Class-F FA and FCA were procured from NTPC Ltd., Talcher, Odisha and Balasore Alloys Ltd., Balasore, respectively. The X-ray fluorescence (XRF) analysis was adopted for FCA and FA to determine their chemical composition (as seen in Table 11.2). It is discerned that FCA holds a major volume of magnesium oxide (MgO)—23.6%, while the other significant

TABLE 11.1 Properties of Ferrochrome Waste-based Geopolymers

Matrix	Binder	Activator	Aggregate	Additive (Conc.)	Curing Conditions	Compressive Strength (MPa)	Key Findings	Refs.
Paste, Mortar	FCS	NaOH + Na_2SiO_3 (Na_2O—7%, Silicate Modulus-0.7), (w/b—0.3)	Quartz Sand	N/A	Ambient Curing, Ambient Curing	7 Day—17.96 28 Day—13.82 7 Day—17.52 28 Day—22.04 90 Day—20.15	FCS-based geopolymers demonstrate higher setting times with lower heat of hydration.	[36, 37]
Concrete	FCS	NaOH (15M) + Na_2SiO_3	River Sand (2–4 mm)	N/A	75°C (72 h) + Ambient Curing + 700°C (1 h)	28 Day—18.92	River sand aggregate-based geopolymer concrete illustrated higher fire resistance against processed sand aggregate geopolymers and cement-based concrete systems.	[38]
Concrete	FCS	NaOH + Na_2SiO_3 (Silicate Modulus—1.35)	River Sand (0–8 mm)	N/A	75°C (72 h) + Ambient Curing	28 Day—35.10 90 Day—32.38 180 Day—31.23	The sulfate resistance of FCS-based geopolymers was slightly higher than OPC-based concrete systems.	[39]
Paste	HCFCS	NaOH (8M) + Na_2SiO_3	N/A	Water Soluble Plasticizer	70°C (24 h) + Ambient Curing	7 Day—11.8 28 Day—14.1	HCFCS-based geopolymers showed stabilization at higher temperatures against the as-received HCFCS.	[40]
Paste	FCS	NaOH (6M) + Na_2SiO_3	N/A	N/A	Ambient Curing	7 Day—26 28 Day—33.8	Higher reactivity of FCS resulted in the development of Ca and Mg-rich hydrated phases, enhancing the strength values.	[41]
Concrete	FA	NaOH (14M) + Na_2SiO_3	River Sand (Zone 3), NCA, FCS	N/A	Ambient Curing (48 h) + 70°C (24 h) + Ambient Curing	7 Day—36.2 28 Day—47.5	Partial application of FCS as coarse aggregate (30%), enhanced all mechanical strength characteristics.	[42]
Paste	FCS	KOH (10M) + KA	N/A	N/A	Ambient Curing	7 Day—9 28 Day—24.2 56 Day—25.1	Aluminate activation of FCS during depolymerization favors strength development against silicate activation.	[43]
Concrete	FCS	NaOH (10M) + Na_2SiO_3 (Silicate Modulus—1.5)	River Sand (0–8 mm)	N/A	80°C (24 h) + Water Curing (23°C)	28 Day—18.14 56 Day—18.17 84 Day—18.38	Acid resistance of geopolymer concrete with FCS is more than geopolymer concrete with BFS, involving H_2SO_4, HF, HCL, and H_3PO_4.	[44]

TABLE 11.1 *(Continued)*

Matrix	Binder	Activator	Aggregate	Additive (Conc.)	Curing Conditions	Compressive Strength (MPa)	Key Findings	Refs.
Concrete	FCA+GGBS	NaOH (12M) + Na_2SiO_3	River Sand (4.75 mm), Crushed Gravel (20 mm)	N/A	Outdoor Curing (O) Ambient Curing (A)	O: 7 Day—29.7 O: 28 Day—30.2 A: 7 Day- N/A A: 28 Day- 17	Although, it was possible to manufacture geopolymer concrete using FCA and GGBS and the strength reached 30.2 MPA under outdoor conditions, all the mixes were very stiff and also resulted in high chromium leaching	[34]
Concrete	FCA+FA	NaOH (12M) + Na_2SiO_3	River Sand (4.75 mm), Crushed Gravel (20 mm)	N/A	Ambient curing	7 Day—9 28 Day—29.3	The combination of FCA and FA (60:40) exhibited better compressive strength (29.3 MPa) under ambient conditions and the chromium leaching was found to be under regulatory limits. Hence, the mix could be used in general construction works and has the potential to replace the cement-based concrete in future.	[45]
Concrete	FCA + GGBFS	NaOH (12M) + Na_2SiO_3	River Sand (4.75 mm), Crushed Gravel (20 mm)	Lime	Outdoor Curing (19–42°C)	7 Day—25 28 Day—27	Introduction of lime in FCA-based geopolymer concrete allowed faster setting time.	[19]
Concrete	FCA + FA	NaOH (13M) + Na_2SiO_3	NCA (10–20 mm), Sand	Super-plasticizer	65°C (24 h) + Ambient Curing	7 Day—20.93 28 Day—29.92 56 Day—32.78	FCA and FA present efficient geopolymerization reaction resulting in enhanced compressive strength values.	[21]
Concrete	FA + SF	NaOH (14M) + Na_2SiO_3	NFA + NCA + FCS	N/A	70°C (24 h) + Ambient Curing	7 Day—42 28 Day—57.5	Density and water absorption of geopolymer concrete reduce with the rise in FCS.	[46]
Concrete	FA + FCA	NaOH + Na_2SiO_3	River Sand (Zone 3), NCA (20 mm)	Super-plasticizer	70°C (24 h) + Ambient Curing	7 Day—31.58 28 Day—33.39	FA- and FCA-based geopolymer concrete exhibited higher compressive strength, flexural and shear failure resistance along with lower deflection and acid resistance, when compared with traditional concrete.	[47]

Note: FCS—Ferrochrome slag, FA—Fly ash, FCA—Ferrochrome ash.

oxides, including aluminum, silicon, iron, and calcium, are present at 10.91%, 19.1%, 7.84%, and 3.14%, respectively. In comparison, FA consists of a high amount of aluminum and silicon oxides (30.85% and 60.35%) with a minor component of calcium oxide (0.81%) which are useful for geopolymerization. The particle size analysis of FCA and FA was conducted using HORIBA LA-960—laser scattering particle size analyzer. Figure 11.2 illustrates the particle size distribution curves for FCA and FA. The details of particle size distribution are as follows: d_{10}—0.33 µm, d_{50}—7.29 µm, and d_{90}—63.29 µm for FCA while d_{10}—4.60 µm, d_{50}—17.71 µm and d_{90}—106.68 µm for FA. This reveals that FCA is finer than the FA. The X-ray diffraction (XRD) analysis using a Rigaku-Ultima-IV X-ray diffractometer was used to evaluate the mineralogical phases present in FCA and FA. Figure 11.3 represents the XRD graphs of FCA and FA. From both the diffractograms, it can be seen that the FA shows a characteristic hump between 20° and 30° (2Θ position) indicating the presence of glassy phases whereas the FCA contains a significant amount of crystalline mineral phases along with amorphous materials. The FA contains quartz and mullite whereas FCA contains phases like forsterite, silvine, hydrotalcite, and donathite. The scanning electron microscope (SEM) images of FCA and FA are presented in Figure 11.4, which reveals that FA and FCA are composed of fine, spherical, porous particles.

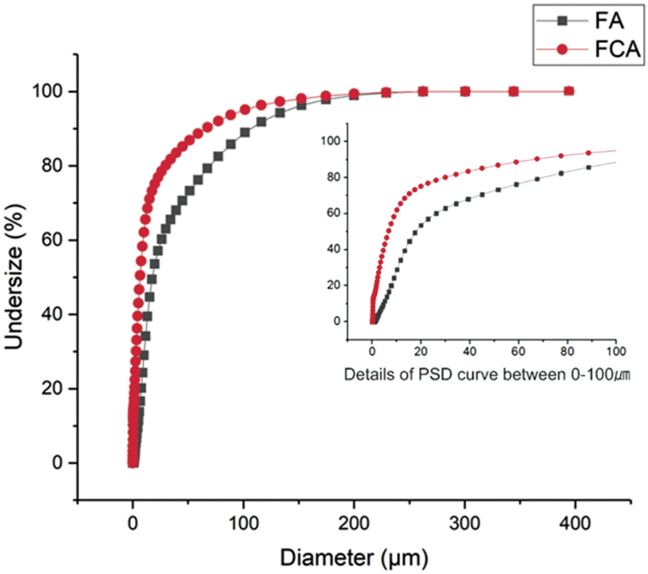

FIGURE 11.2 Particle size distribution curve of FCA and FA. ⏎

Source: Reprinted from Ref. [45].

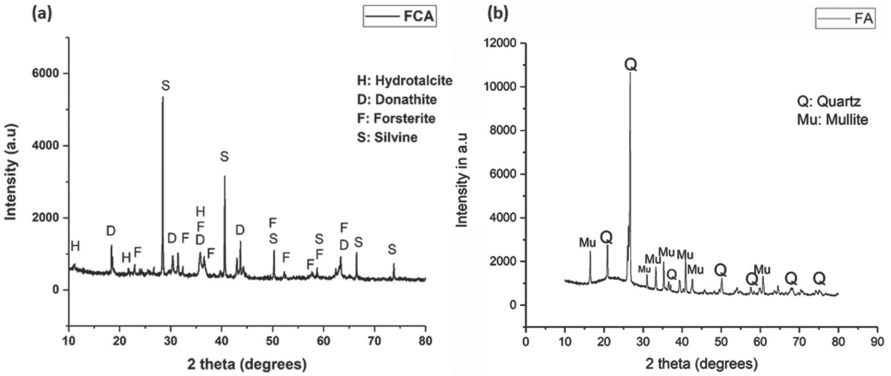

FIGURE 11.3 XRD diffractograms of (a) FCA, (b) FA. ⏎

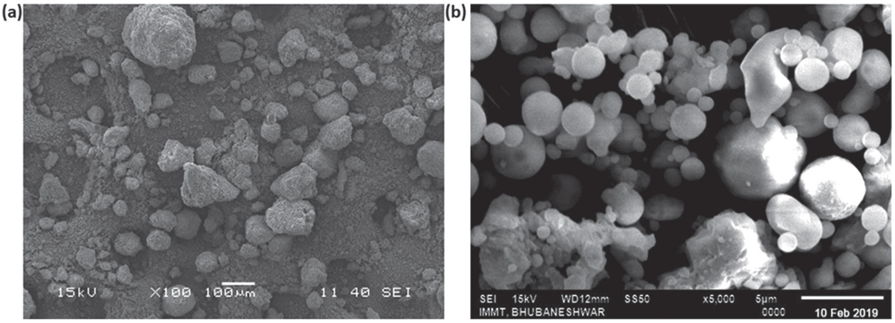
(a)
15kU ×100 100µm 11 40 SEI
(b)
SEI 15kV WD12mm SS50 x5,000 5µm
IMMT, BHUBANESHWAR 0000 10 Feb 2019

FIGURE 11.4 SEM micrographs of (a) FCA (b) FA [45]. ⏎

Source: Reprinted from Ref. [45].

The alkaline solution used for geopolymerization plays a crucial part during the strength evolution. Hence, a mixture of NaOH and Na_2SiO_3 solutions has been implemented for this study. The locally obtainable NaOH flakes (98% purity) and Na_2SiO_3 solution (32.15%—SiO_2, 15.85%—Na_2O, and 52%—H_2O by mass) were used for this study.

Furthermore, commercially available hydrated lime was used to prepare saturated lime water. For this, 50 g of hydrated lime was dissolved into water (1 L), subjected to stirring, and left to sediment for 24 h. After that, only the top layer of the solution was used during the concrete preparation as the solid particles of hydrated lime settled on the bottom. Naturally available river sand (4.75 mm IS sieve passing) and crushed gravel of 20 mm downsize were obtained from local suppliers and were utilized as fine and coarse aggregates, respectively.

TABLE 11.2 Chemical Constituents of Source Materials Detected from XRF Analysis [45] ⏎

Materials	SiO_2	Al_2O_3	CaO	MgO	Fe_2O_3	K_2O	Na_2O	P_2O_5	TiO_2	Cr_2O_3
FCA	19.10	10.91	3.14	23.60	7.84	11.42	2.46	0.07	0.13	9.89
FA	60.35	30.85	0.81	0.548	3.35	1.27	0.09	0.53	1.88	0.03

11.2.2 MIXING, CASTING, AND CURING

This study used a predetermined mixture proportion of 1:1:3 by weight to prepare the geopolymer concrete mixes. In total, three different geopolymer concrete mixes, namely, FCA40FA60, FCA60FA40, and FCA80FA20, were designed where the numbers in the mix designations suggest the percentage of utilized source materials. Past works of the authors [19, 20, 48, 49] indicate that 12 M NaOH mixed with Na_2SiO_3 (1:2 by volume) provides better strength development. Hence for this study, the concentration of 12 M NaOH solution was blended with $NaSi_2O_3$ solution at 1:2 by volume. The activator was made 30 minutes before experimentation. Mix design for the preparation of 1 m^3 of geopolymer concrete is depicted in Table 11.3.

TABLE 11.3 Mix Design for 1 m^3 of FCA-based Geopolymer Concrete with FA and Lime Water ⏎

Mix No.	FCA (kg/m^3)	FA (kg/m^3)	Fine Aggregate (kg/m^3)	Coarse Aggregate (kg/m^3)	Sodium Hydroxide (L/m^3)	Sodium Silicate (L/m^3)	Lime Water (L/m^3)
FCA40FA60	200.00	300.00	1500.00	500.00	50.00	100.00	20.00
FCA60FA40	300.00	200.00	1500.00	500.00	50.00	100.00	20.00
FCA80FA20	400.00	100.00	1500.00	500.00	50.00	100.00	20.00

The mixing process includes dry mixing and wet mixing of the ingredients. The source materials were mixed with the aggregates in their dry states, and then wet mixing was done, that is after the introduction of alkaline solution and lime water (300 mL), to form a homogenous geopolymer concrete mixture. Subsequently, the concrete mix, after 11 minutes of thorough mixing, was poured into 150 × 150 × 150 mm mold for casting and subjected to vibrations for 2 min. The curing was done at room temperature conditions (temperature: 24±3°C, relative humidity: 90%). A flowchart is shown in Figure 11.5, representing the experimental procedure.

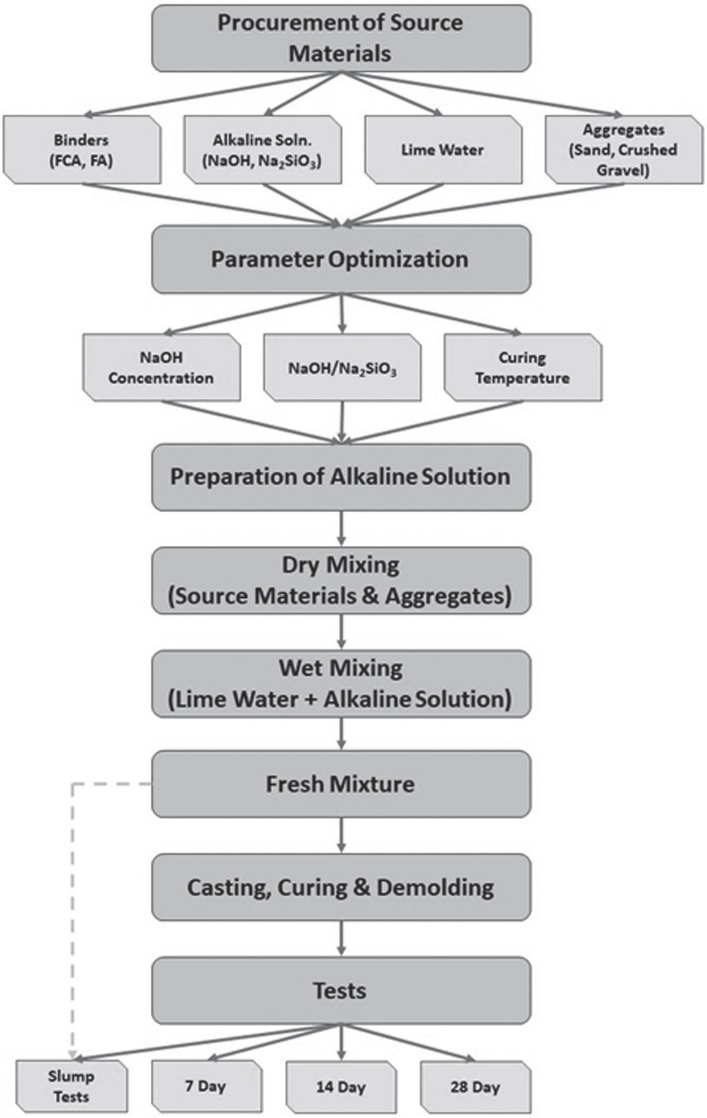
Procurement of Source Materials
Binders (FCA, FA)
Alkaline Soln. (NaOH, Na_2SiO_3)
Lime Water
Aggregates (Sand, Crushed Gravel)
Parameter Optimization
NaOH Concentration
NaOH/Na_2SiO_3
Curing Temperature
Preparation of Alkaline Solution
Dry Mixing (Source Materials & Aggregates)
Wet Mixing (Lime Water + Alkaline Solution)
Fresh Mixture
Casting, Curing & Demolding
Tests
Slump Tests
7 Day
14 Day
28 Day

FIGURE 11.5 Flowchart for the experimental work. ⏎

11.2.3 TEST METHODS

The testing methods implemented to realize the performance of the resulting concrete are: (1) Workability test (IS-1199:1959), and (2) compressive strength test at the age of 7, 14, and 28 days (IS-516:1959) with the help of a 2000 kN compression testing machine (CTM).

11.3 RESULTS AND DISCUSSIONS

11.3.1 SLUMP

In geopolymer concrete production, the slump test can provide important information about the degree of fluidity and mobility of a geopolymer concrete mix. The workability test for the fresh geopolymer concrete mixes incorporating FA and lime water was carried out through the method of the slump-cone test (IS-1199:1959). The slumps associated with the three mixes (FCA40FA60, FCA60FA40, FCA80FA20) were presented in Table 11.4. The slump test values revealed that there were three kinds of slump achieved; collapse, true, and zero. The mix FCA60FA40 exhibited a true slump of 55 mm, which could be suitable for general construction applications without the need for any superplasticizers. In contrast, in FCA40FA60 and FCA80FA20, the slump cone procedure showed collapse and zero slumps, respectively.

TABLE 11.4 Workability of the FCA-Based Geopolymer Concrete Mixes ⏎

Mix No.	Slump Type and Value (mm)
FCA40FA60	Collapse
FCA60FA40	True slump (55 mm)
FCA80FA20	Zero slump

At the time of laboratory testing, the slump of the mix FCA40FCA60 collapsed within a short span after the slump cone was lifted. The reason could be assigned to the excessive water content inside the system. As the amount of FA is higher, free water expulses due to the geopolymerization of aluminosilicate compounds. Moreover, the water content from the lime water also increases water-geopolymer solids ratio. Thus, the fluidity of the mixes could have increased and caused segregation leading to a collapsed slump. This also reveals that the slump test for this mix is unfavorable. It is recommended to utilize the flow test method to determine workability in future works.

On the other hand, the mix FCA60FA40 showed a slump of 55 mm and the reason is ascribed to the blended influence of spherical-shaped FA and

FCA particles, which acted as ball bearings [48, 50, 51] along with the lubrication provided by the sodium silicate solution resulting in a definite slump (55 mm). Moreover, the total water content provided by the addition of lime water and the overall geopolymerization process also aided in improving the slump.

Contrary to the earlier results, the mix FCA80FA20 demonstrated zero slump. The concrete mix was found to be harsh, stiff, and with dry consistency immediately after removing the slump cone. This suggests that there was a shortage of water in the mix. Also, the FA content is less than other mixes; hence less amount of aluminosilicate compounds led to reduced free water expulsion from ineffective geopolymerization. The unavailability of free water decreased the fluidity of the mix. One more reason could be as a result of increased fineness and specific surface area of FCA particles that probably consumed water from the system leading to a dry mix with zero slump. However, the concrete mix with zero slumps can be effectively used in pre-fabrication industries requiring less reinforcement.

11.3.2 COMPRESSIVE STRENGTH

Three specimens were cast in each case (FCA40FA60, FCA60FA40, FCA80FA20), resulting in total of nine geopolymer cube specimens and subjected to a CS test under a 2000 kN testing machine. The average CS test results at 7, 14, and 28 days are depicted in Figure 11.6.

FCA60FA40 achieved the maximum CS of 21 MPa at 28 days, whereas mix FCA80FA20 attained the minimum CS of 11 MPa (*as seen* in Figure 11.6). Besides, it is noted that there is a notable increment in the strength development of 7- and 28-day-aged specimens in all of the mixes, which suggests geopolymerization increases with time. Compared to the mix FCA40FA60, there is a rise in 28-day CS by 20 % when FCA content is increased (FCA60FA40 mix). However, increasing the FA content by 20 %, as in the case of FCA80FA40, it is noticed that there is a significant reduction in 28-day CS by 47.6 % in comparison to the FCA60FA40.

Strength development in FA-based geopolymer mixes is primarily ascribed to the development of N-A-S-H type gels [52–54] in the evolution of a solid geopolymer network. This is noticed in this study. Moreover, the calcium from the source materials (3.14% and 0.81%) and saturated lime water are equally accountable for the generating C-S-H and C-A-S-H gel; thus, offering an overall strength gain of all mixes at various curing ages. Together, these geopolymer gels influenced the strength gain of the ambient cured samples. Extra calcium imparted from lime water during mixing also aided in reducing the setting process and enhancing the reaction rate at room temperature conditions. The cube specimens could be easily molded (as shown in Figure 11.7) after 24 h, thus requiring the need for any rest period for setting purposes. Furthermore, it is likely that the alkalinity increased when saturated lime water was added, for which the dissolution rate of aluminum and silicon might have significantly improved and led to gradual development in the CS over the ages.

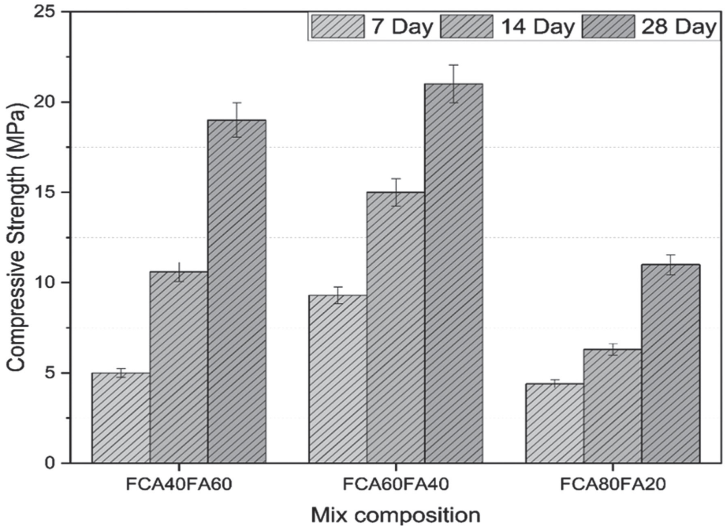

FIGURE 11.6 Compressive strength FCA–FA geopolymer concrete with lime water at 7, 14, and 28 days. ⏎

When compared with the results of past studies, it is observed that the inclusion of lime water instead of potable water can also have negative effects on compressive strength development. In one study [45], the authors investigated the geopolymerization potential of blending FCA along with FA under ambient curing conditions. The highest compressive strength of 29.3 MPa was attained by the mix containing FCA 60% and FA 40%. It is worthwhile to note that the trend of compressive strength development is similar in both studies. However, in comparison, a strength reduction of 28% at 28 days is noticed when lime water is used for mixing purposes. This indicates that the inclusion of lime water during mixing reduces the compressive strength drastically. It establishes the fact that the use of lime water may not be suitable for all types of geopolymer concrete, as it can react differently with different types of aluminosilicate precursors [55–57]. The actual reasons for strength reduction remain a matter of scope of research.

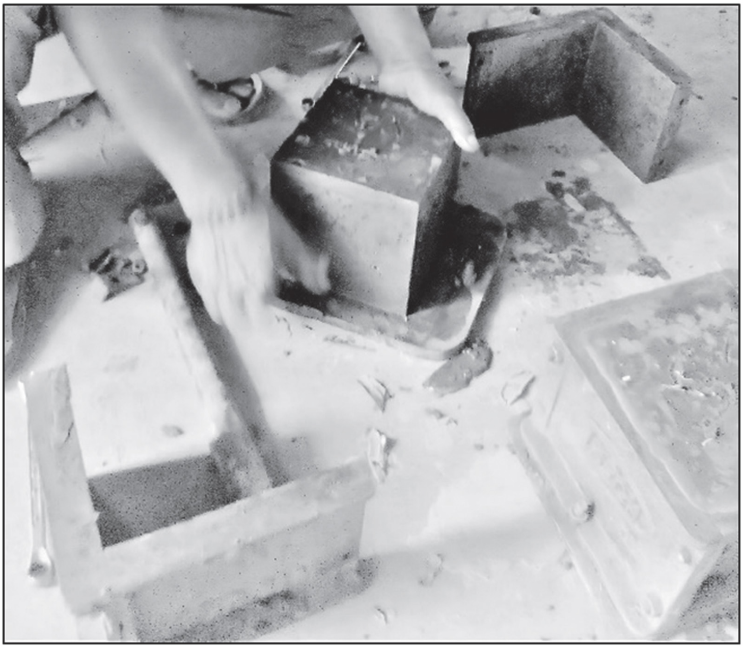

FIGURE 11.7 The demolding of cube specimens after 24 h. ⏎

Apart from FA, the existence of FCA in the system is vital with respect to strength development. Although FCA has less amount of aluminum and silicon oxides, it has a significant quantity of magnesium oxide (MgO), that is, 23.6%, which seems to dominate the strength development process in the case of FCA60FA40 mix by the development of hydrotalcite-like phases leading to the highest strength among the other mixes. The past literature has indicated that the high content of MgO in the mix spawned a substantial increment in CS by reducing the porosity.

However, the excess of MgO could potentially reduce the strength, as revealed from past studies [58]. Excessive amounts of MgO can result in an excessively high pH, which can lead to issues such as delayed setting and reduced strength development. This behavior is confirmed in the case of the FCA80FA20 mix of the present study, where the strength was reduced at 28 days. This reduction might be because of insufficient aluminosilicate compounds in the mix, as FA content is low (20%), for which the geopolymerization was less prominent.

11.4 SCOPE OF FUTURE RESEARCH

This study discussed the workability and compressive strength of FCA–FA-based geopolymer concrete where lime water was used as mixing water. It is seen that the strength development was found to be low when compared with geopolymer concrete mixes prepared using potable water. This suggests that there is a need for further investigation to determine the exact causes of strength reduction. Accordingly, some of the scope of future research is highlighted below:

- The mineralogical phases of the hardened concrete samples may be checked using XRD analysis. This shall reveal the crystalline phases present in the matrix after geopolymerization and aid in comprehending the reasons for the decrement in strength.
- SEM analysis may be done to assess the morphological characteristics of the matrix so as to deduce the causes for strength reduction when lime water is used.
- More number of experiments may be done with variable lime water content to determine the variation in strength properties and reach an optimum limit of lime water content.
- The investigation on the use of superplasticizers to enhance the slump of the mixes may be carried out so that the scope of applications shall be widened for different concrete works.
- Addition of additives such as rice husk ash and silica fume to improve the strength may be adopted that satisfies the standards of M20 grade concrete.

11.5 CONCLUSIONS

This study details the results from the investigation on using lime water to prepare geopolymer concrete under room temperature conditions using FCA and FA. The addition of 40% FA to the matrix system notably improves the slump and CS properties. The mix FCA60FA40 showed the highest slump (55 mm) and achieved the maximum 28-day CS of 21 MPa. CS reduced when FCA content was 80% of the source material composition (FCA80FA20) due to the impact of excess magnesium oxide. The extra calcium content in the form of lime water may have aided in the generation of C-S-H gel which, in conjunction with N-A-S-H, promoted strength evolution. However, in comparison, it is found that the inclusion of lime water drastically reduces the 28-day compressive strength for the same mix that used potable water under ambient curing conditions. It was hypothesized that lime water could help in improving the compressive strength by increasing the alkalinity of the mix, but the results did not comply with the hypothesis. Further studies are therefore required to determine the exact causes of this reduction and to figure out the right quantity of lime water to be used in the manufacturing of FCA–FA-based geopolymer concrete.

KEYWORDS

- **fly ash**
- **ferrochrome ash**
- **lime**
- **geopolymer concrete**
- **workability**
- **compressive strength**

REFERENCES

1. Gartner, E. Industrially interesting approaches to "Low-CO_2" cements. *Cem. Concr. Res.*, **2004**, *34*, 1489–1498, https://doi.org/10.1016/j.cemconres.2004.01.021.
2. Das, S.K., Krishna, R.S., Mishra, S., Mustakim, S.M., Jena, M.K., Tripathy, A.K., Sahu, T. Future trends. In *Handbook of sustainable concrete and industrial waste management*, Elsevier, 2022, pp. 529–550.
3. Krishna, R.S., Mishra, J., Das, S.K., Nanda, B., Patro, S.K., Mustakim, S.M. *A review on potential of graphene reinforced geopolymer composites*. In *Tailored functional materials*, 2022, pp. 43–60.
4. Mishra, J., Nanda, B., Patro, S.K., Krishna, R.S. Sustainable fly ash based geopolymer binders: a review on compressive strength and microstructure properties. *Sustainability*, **2022**, *14*, 15062, https://doi.org/10.3390/su142215062.
5. Lecomte, I., Henrist, C., Liégeois, M., Maseri, F., Rulmont, A., Cloots, R. (Micro)-structural comparison between geopolymers, alkali-activated slag cement and portland cement. *J. Eur. Ceram. Soc.*, **2006**, *26*, 3789–3797, https://doi.org/10.1016/j.jeurceramsoc.2005.12.021.

6. Duxson, P., Fernández-Jiménez, A., Provis, J.L., Lukey, G.C., Palomo, A., van Deventer, J.S.J. Geopolymer technology: the current state of the art. *J. Mater. Sci.*, **2007**, *42*, 2917–2933, https://doi.org/10.1007/s10853-006-0637-z.
7. Lee, W.K.W., van Deventer, J.S.J. The effect of ionic contaminants on the early-age properties of alkali-activated fly ash-based cements. *Cem. Concr. Res.*, **2002**, *32*, 577–584, https://doi.org/10.1016/S0008-8846(01)00724-4.
8. Hassan, A., Arif, M., Shariq, M. Influence of microstructure of geopolymer concrete on its mechanical properties—a review. In *Advances in sustainable construction materials and geotechnical engineering,* 2020, pp 119–129.
9. Marjanović, N., Komljenović, M., Baščarević, Z., Nikolić, V. Comparison of two alkali-activated systems: mechanically activated fly ash and fly ash-blast furnace slag blends. *Procedia. Eng.*, **2015**, *108*, 231–238, https://doi.org/10.1016/j.proeng.2015.06.142.
10. Sikder, A., Mishra, J., Krishna, R.S., Ighalo, J.O. Evaluation of the mechanical and durability properties of geopolymer concrete prepared with C-glass fibers. *Arab. J. Sci. Eng.*, **2022**, https://doi.org/10.1007/s13369-022-07558-y.
11. Aziz, A., Stocker, O., el Amrani El Hassani, I.-E., Laborier, A.P., Jacotot, E., el Khadiri, A., el Bouari, A. Effect of blast-furnace slag on physicochemical properties of pozzolan-based geopolymers. *Mater. Chem. Phys.*, **2021**, *258*, 123880, https://doi.org/10.1016/j.matchemphys.2020.123880.
12. Talaat, A., Emad, A., Kohail, M. Environmental impact assessment for performance-oriented geopolymer concrete research. *J. Mater. Civ. Eng.*, **2023**, *35*, https://doi.org/10.1061/(ASCE)MT.1943-5533.0004526.
13. Acharya, P.K., Patro, S.K. Strength, sorption and abrasion characteristics of concrete using ferrochrome ash (FCA) and lime as partial replacement of cement. *Cem. Concr. Compos.*, **2016**, *74*, 16–25, https://doi.org/10.1016/j.cemconcomp.2016.08.010.
14. Acharya, P.K., Patro, S.K. Acid resistance, sulphate resistance and strength properties of concrete containing ferrochrome ash (FA) and lime. *Constr. Build. Mater.*, **2016**, *120*, 241–250, https://doi.org/10.1016/j.conbuildmat.2016.05.099.
15. Acharya, P.K., Patro, S.K. Utilization of ferrochrome wastes such as ferrochrome ash and ferrochrome slag in concrete manufacturing. *Waste Manag. Res.*, **2016**, *34*, 764–774, https://doi.org/10.1177/0734242X16654751.
16. Acharya, P.K., Patro, S.K. Use of ferrochrome ash (FCA) and lime dust in concrete preparation. *J. Clean. Prod.*, **2016**, *131*, 237–246, https://doi.org/10.1016/j.jclepro.2016.05.042.
17. Kumar, B.A.V.R., Keshav, L., Sivanantham, P.A., Arokiaraj, G.G.V., Rahman, D.R.Z., Kumar, P.M., Somashekar, D. Comprehensive characterization of ferrochrome slag and ferrochrome ash as sustainable materials in construction. *J. Nanomater.*, **2022**, *2022*, 1–12, https://doi.org/10.1155/2022/8571055.
18. Kumar B.C., Yaragal, S.C., Das, B.B. Ferrochrome ash—its usage potential in alkali activated slag mortars. *J. Clean. Prod.*, **2020**, *257*, 120577, https://doi.org/10.1016/j.jclepro.2020.120577.
19. Mishra, J., Kumar Das, S., Krishna, R.S., Nanda, B., Kumar Patro, S., Mohammed Mustakim, S. Synthesis and characterization of a new class of geopolymer binder utilizing ferrochrome ash (FCA) for sustainable industrial waste management. *Mater. Today. Proc.*, **2020**, *33*, 5001–5006, https://doi.org/10.1016/j.matpr.2020.02.832.
20. Mishra, J., Das, S.K., Krishna, R.S., Nanda, B. Utilization of ferrochrome ash as a source material for production of geopolymer concrete for a cleaner sustainable environment. *Indian Concr. J.*, **2020**, *94*, 40–49.

21. Saha, S., Mohanty, T., Saha, P. Mechanical Properties of fly ash and ferrochrome ash-based geopolymer concrete using recycled aggregate. In *Recent developments in sustainable infrastructure, select proceedings of ICRDSI 2019*. 2021, pp. 417–426.
22. Diaz, E.I., Allouche, E.N., Eklund, S. Factors affecting the suitability of fly ash as source material for geopolymers. *Fuel*, **2010**, *89*, 992–996, https://doi.org/10.1016/j.fuel.2009.09.012.
23. Fernandez-Jimenez, A., García-Lodeiro, I., Palomo, A. Durability of alkali-activated fly ash cementitious materials. *J. Mater. Sci.*, **2007**, *42*, 3055–3065, https://doi.org/10.1007/s10853-006-0584-8.
24. Guo, X., Shi, H., Chen, L., Dick, W.A. Alkali-activated complex binders from class C fly ash and Ca-containing admixtures. *J. Hazard. Mater.*, **2010**, *173*, 480–486, https://doi.org/10.1016/j.jhazmat.2009.08.110.
25. Temuujin, J., van Riessen, A., Williams, R. Influence of calcium compounds on the mechanical properties of fly ash geopolymer pastes. *J. Hazard. Mater.* **2009**, *167*, 82–88, https://doi.org/10.1016/j.jhazmat.2008.12.121.
26. Hake, S.L., Damgir, R.M., Patankar, S.V. Temperature effect on lime powder-added geopolymer concrete. *Adv. Civ. Eng.*, **2018**, *2018*, 1–5, https://doi.org/10.1155/2018/6519754.
27. Rashad, A.M. A comprehensive overview about the influence of different admixtures and additives on the properties of alkali-activated fly ash. *Mater. Des.*, **2014**, *53*, 1005–1025, https://doi.org/10.1016/j.matdes.2013.07.074.
28. Richardson, I.G., Brough, A.R., Groves, G.W., Dobson, C.M. The characterization of hardened alkali-activated blast-furnace slag pastes and the nature of the calcium silicate hydrate (C-S-H) phase. *Cem. Concr. Res.*, **1994**, *24*, 813–829, https://doi.org/10.1016/0008-8846(94)90002-7.
29. Abd Elaty, M.A.A., Ghazy, M.F. Performance of portland cement mixes containing silica fume and mixed with lime-water. *HBRC J.*, **2014**, *10*, 247–257, https://doi.org/10.1016/j.hbrcj.2013.12.004.
30. Solikin, M., Setunge, S., Patnaikuni, I. Experimental design analysis of ultra fine fly ash, lime water, and basalt fibre in mix proportion of high volume fly ash concrete. *Pertanika. J. Sci. Technol.*, **2013**, *21*, 589–600.
31. Ling, X., Setunge, S., Patnaikuni, I. Effect of different concentrations of lime water on mechanical properties of high volume fly ash concrete. In *From materials to structures: advancement through innovation*, CRC Press, 2012, pp. 1135–1141.
32. Mishra, J., Kumar Das, S., Krishna, R.S., Nanda, B., Kumar Patro, S., Mohammed Mustakim, S. Synthesis and characterization of a new class of geopolymer binder utilizing ferrochrome ash (FCA) for sustainable industrial waste management. *Mater. Today. Proc.*, **2020**, 6–11, https://doi.org/10.1016/j.matpr.2020.02.832.
33. Mishra, J., Das, S.K., Krishna, R.S., Nanda, B. Utilization of ferrochrome ash as a source material for production of geopolymer concrete for a cleaner sustainable environment. *Indian Concr. J.*, **2020**, *94*, 40–49.
34. Mishra, J., Nanda, B., Patro, S.K., Das, S.K., Mustakim, S.M. Influence of ferrochrome ash on mechanical and microstructure properties of ambient cured fly ash-based geopolymer concrete. *J. Mater. Cycles. Waste. Manag.*, **2022**, *24*, 1095–1108, https://doi.org/10.1007/s10163-022-01381-1.
35. Kumar B, C., Yaragal, S.C., Das, B.B. Ferrochrome ash – its usage potential in alkali activated slag mortars. *J. Clean. Prod.*, **2020**, *257*, https://doi.org/https://doi.org/10.1016/j.jclepro.2020.120577.

36. Karakoc, M.B., Kantarci, F., Turkmen, I., Demirboga, R., Maras, M.M., Toprak, M.U. Mechanical properties and setting time of geopolymer paste and mortar produced from ferrochrome slag. In *Proceedings of the 2013 International Conference on Renewable Energy Research and Applications (ICRERA)*, IEEE, October 2013, pp. 52–57.
37. Karakoç, M.B., Türkmen, İ., Maraş, M.M., Kantarci, F., Demirboğa, R., Uğur Toprak, M. Mechanical properties and setting time of ferrochrome slag based geopolymer paste and mortar. *Constr. Build. Mater.*, **2014**, *72*, 283–292, https://doi.org/10.1016/j.conbuildmat.2014.09.021.
38. Türkmen, İ., Karakoç, M.B., Kantarcı, F., Maraş, M.M., Demirboğa, R. Fire resistance of geopolymer concrete produced from Elaziğ ferrochrome slag. *Fire. Mater.*, **2016**, *40*, 836–847, https://doi.org/10.1002/fam.2348.
39. Karakoç, M.B., Türkmen, İ., Maraş, M.M., Kantarci, F., Demirboğa, R. Sulfate resistance of ferrochrome slag based geopolymer concrete. *Ceram. Int.*, **2016**, *42*, 1254–1260, https://doi.org/10.1016/j.ceramint.2015.09.058.
40. Panigrahi, M., Mohanty, S., Ganguly, R.I., Dash, R.R. An advanced cured High Carbon Ferrochrome Slag (HCFCS) Geopolymer (GP): a constructional materials. *IOP Conf. Ser. Mater. Sci. Eng.*, **2018**, *410*, 012002, https://doi.org/10.1088/1757-899X/410/1/012002.
41. Nath, S.K. Geopolymerization behavior of ferrochrome slag and fly ash blends. *Constr. Build. Mater.*, **2018**, *181*, 487–494, https://doi.org/10.1016/j.conbuildmat.2018.06.070.
42. Jena, S., Panigrahi, R. Performance assessment of geopolymer concrete with partial replacement of ferrochrome slag as coarse aggregate. *Constr. Build. Mater.*, **2019**, *220*, 525–537, https://doi.org/10.1016/j.conbuildmat.2019.06.045.
43. Falayi, T. Sustainable solidification of ferrochrome slag through geopolymerisation: a look at the effect of curing time, type of activator and liquid solid ratio. *Sustain. Environ. Res.*, **2019**, *29*, 21, https://doi.org/10.1186/s42834-019-0022-7.
44. Özcan, A., Karakoç, M.B. The resistance of blast furnace slag- and ferrochrome slag-based geopolymer concrete against acid attack. *Int. J. Civ. Eng.*, **2019**, *17*, 1571–1583, https://doi.org/10.1007/s40999-019-00425-2.
45. Mishra, J., Nanda, B., Patro, S. K., Das, S. K., Mustakim, S. M. Influence of ferrochrome ash on mechanical and microstructure properties of ambient cured fly ash-based geopolymer concrete. *J Mater Cycles Waste Manag.*, **2022**, *24*(3), 1095–1108. https://doi.org/10.1007/s10163-022-01381-1
46. Jena, S., Panigrahi, R. Feasibility study of the properties of geopolymer concrete with ferrochrome slag and silica fume. *Mater. Today. Proc.*, **2021**, *38*, 2476–2480, https://doi.org/10.1016/j.matpr.2020.07.510.
47. Mohanty, T., Kumar, A., Acharya, P.K., Patro, S.K., Saha, P. Performance of structural geopolymer concrete utilising ferrochrome ash and fly ash as source material. *J. Inst. Eng. (India): A*, **2022**, https://doi.org/10.1007/s40030-022-00681-x.
48. Mustakim, S.M., Das, S.K., Mishra, J., Aftab, A., Alomayri, T.S., Assaedi, H.S., Kaze, C.R. Improvement in fresh, mechanical and microstructural properties of fly ash- blast furnace slag based geopolymer concrete by addition of nano and micro silica. *Silicon*, **2021**, *13*, 2415–2428, https://doi.org/10.1007/s12633-020-00593-0.
49. Das, S.K., Mustakim, S.M., Adesina, A., Mishra, J., Alomayri, T.S., Assaedi, H.S., Kaze, C.R. Fresh, strength and microstructure properties of geopolymer concrete incorporating lime and silica fume as replacement of fly ash. *J. Build. Eng.*, **2020**, *32*, 101780, https://doi.org/10.1016/j.jobe.2020.101780.

50. Provis, J.L., Duxson, P., van Deventer, J.S.J. The role of particle technology in developing sustainable construction materials. *Adv. Powder. Technol.*, **2010**, *21*, 2–7, https://doi.org/10.1016/j.apt.2009.10.006.
51. Duxson, P., Provis, J.L. Designing precursors for geopolymer cements. *J. Am. Ceram. Soc.*, **2008**, *91*, 3864–3869, https://doi.org/10.1111/j.1551-2916.2008.02787.x.
52. Garcia-Lodeiro, I., Fernandez-Jimenez, A., Palomo, A. Hydration kinetics in hybrid binders: early reaction stages. *Cem. Concr. Compos.*, **2013**, *39*, 82–92, https://doi.org/10.1016/j.cemconcomp.2013.03.025.
53. Luhar, S., Chaudhary, S., Luhar, I. Thermal resistance of fly ash based rubberized geopolymer concrete. *J. Build. Eng.*, **2018**, *19*, 420–428, https://doi.org/10.1016/j.jobe.2018.05.025.
54. Ismail, I., Bernal, S.A., Provis, J.L., San Nicolas, R., Hamdan, S., van Deventer, J.S.J. Modification of phase evolution in alkali-activated blast furnace slag by the incorporation of fly ash. *Cem. Concr. Compos.*, **2014**, *45*, 125–135, https://doi.org/ 10.1016/j.cemconcomp.2013.09.006.
55. Lee, W.-H., Lin, K.-L., Chang, T.-H., Ding, Y.-C., Cheng, T.-W. Sustainable development and performance evaluation of marble-waste-based geopolymer concrete. *Polymers (Basel)*, **2020**, *12*, 1924, https://doi.org/10.3390/polym12091924.
56. Zhao, R., Sanjayan, J.G. Geopolymer and portland cement concretes in simulated fire. *Mag. Concr. Res.*, **2011**, *63*, 163–173, https://doi.org/10.1680/macr.9.00110.
57. Wang, W.-C., Wang, H.-Y., Tsai, H.-C. Study on engineering properties of alkali-activated ladle furnace slag geopolymer. *Constr. Build. Mater.*, **2016**, *123*, 800–805, https://doi.org/10.1016/j.conbuildmat.2016.07.068.
58. Li, Z., Zhang, W., Wang, R., Chen, F., Jia, X., Cong, P. Effects of reactive MgO on the reaction process of geopolymer. *Materials*, **2019**, *12*, 526, https://doi.org/10.3390/ma12030526.

PART III
Applications of Smart Materials

CHAPTER 12

TRENDS IN ROBOTICS TECHNOLOGY: SOLUTION FOR MATERIALS TO MANUFACTURING

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ABSTRACT

Most certainly, the industry of robots has created many ways to make human life more easy and quick. The technology of robotics plays an important role in medical fields; the fields of robotics have a great work in manufacturing sector. These machines design the things accurately and these technologies are far more fast and accurate than humans. Various Robots Technologies are appearing everywhere in the society. In this chapter, we have researched about technology of different types of robots and various materials used in manufacturing of robots are also explored. Material properties significantly affect the overall efficiency of robots, such as steel and special aluminum provide good strength to the robot body. The concept of regenerative charge

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has been proposed in this chapter and about unique survival technologies (especially in defence sector) for hybrid robots. With unique upgrades in the framework and sensors the technology use after a collision or how the robots can be prepared to survive in different parameters and various deployable techniques for the robots are discussed. This work gives an elaborated view of emerging technology in robot and the challenges due to different parameters like materials used in designing, sensors, motors, etc.

12.1 INTRODUCTION

Within the past few decades, mechanical technology has changed from a specialty field to a standard innovation that touches nearly every viewpoint of our lives. From fabricating to healthcare, instruction to amusement, mechanical autonomy has revolutionized the way we live, work, and are associated with machines. There are different sorts of mechanical innovations accessible nowadays, each with one-of-a-kind highlights and applications [1].

To begin with, let us take a look at various details about the mechanical robots. Mechanical robots are commonly utilized in fabricating and generation lines to robotize monotonous assignments such as welding, portray, get together, and bundling. These robots are regularly expansive and have a few tomahawks of development, permitting them to perform assignments with exactness and speed. Mechanical robots have revolutionized the fabricating industry, making it more productive, secure, and cost-effective. They have too permitted producers to create higher quality items with fewer errors and squander [2].

Benefit robots are outlined to help individuals in different settings, such as healing centers, homes, and open spaces. These robots can perform a wide run of assignments, from cleaning and upkeep to conveyance and transportation. Service robots have gotten to be progressively well-known in healthcare, where they are utilized to help with quiet care, medicine administration, and restoration. They are moreover commonly utilized in hospitality and retail businesses to supply client benefit, excitement, and help [3].

Versatile robots are another sort of mechanical innovation that has picked up ubiquity in recent years. These robots are prepared with wheels or legs, permitting them to move around and explore diverse situations. Versatile robots can be utilized for different purposes, such as investigating space, performing look and protect missions, and conveying merchandise. They can also be utilized in farming to monitor crops and animals, and in development to help with building and support assignments [4].

Collaborative robots or cobots, are outlined to work nearby people, sharing errands and workspace. Cobots are ordinarily smaller and more lightweight than mechanical robots, and they are prepared with sensors and security highlights to guarantee they can work securely near people. Cobots have gotten to be prevalent in fabricating and gathering lines, where they can work nearby people to perform errands that require accuracy and dexterity [5].

At last, we have independent robots. Independent robots are planned to function autonomously, without human intercession. These robots are regularly prepared with sensors, cameras, and other innovations that allow them to explore and associate with their environment. Independent robots can be utilized in different applications, such as transportation, exploration, and observation. They are moreover utilized within the military for surveillance and bomb transfer [6].

The field of mechanical autonomy has come a long way in the past few decades, and there are presently different sorts of automated innovations accessible to suit diverse applications and needs. Mechanical robots have revolutionized fabricating, benefit robots are being utilized to help individuals in different settings, versatile robots are allowing us to investigate unused wildernesses, collaborative robots are working nearby people to progress productivity and security, and independent robots are working autonomously to solve complex issues. As innovation proceeds to advance, we anticipate to see indeed more energizing headways within the field of mechanical technology. In this work, we are going investigate a few of the foremost well-known sorts of automated innovations and their individual functionalities in the field of robotics technology. This chapter also describes about the availability of different materials used in robot designing with the challenges for future.

12.2 BACKGROUND STUDY

Automated unmanned machines will lead the way by acting as the building blocks of the future. They will play a vital role in Industry 4.0. Robots are adaptable devices capable of carrying out difficult manipulation operations, they are now used in a range of manufacturing processes because of recent advancements in industrial robotics. Recent initiatives have shown how robots can be utilized in additive manufacturing (AM) procedures [7].

Recent initiatives have shown how robots can be utilized in AM procedures. AM advances (too known as quick prototyping, 3D printing, strong freeform manufacture, etc.) have been made for more than 30 years. As AM has progressed, it has been utilized in an assortment of businesses, including aviation, medication, development, and buyer products. AM utilizes an added substance prepared to make things from the bottom up in a point-by-point and after that layer-by-layer procedure, in differentiate from ordinary subtractive fabricating, which employments a subtractive strategy (such as tooling and cutting). The seven essential categories of AM innovation utilized nowadays are sheet cover, fabric expulsion, fabric flying, powder bed fusion, binder jetting, vat photopolymerization, and coordinated vitality statement.

To form the ultimate item, each of these seven AM techniques—material expulsion, fabric flying, powder bed combination, cover streaming, vat photopolymerization, and coordinated vitality deposition—requires a testimony way that takes after the 3D demonstration. Way arranging is the term utilized in AM to depict the method of planning the ways for fabricating. Since changed way methods can affect surface roughness, dimensional precision, and the properties (like quality) of the printed objects, way arranging is pivotal in added substance fabricating. Too, diverse pathways result in completely different moving strategies for the associated print head (for case, the spout in fused deposition modeling, or the laser in direct energy deposition), which comes about in different turnaround times for the same object [7, 8].

A much better, higher, stronger, and improved way of arranging procedures can subsequently result in higher manufactured quality, properties, or a shorter creation time. There are presently a few considerations on this subject that have been distributed. Modern added substance fabricating advances are being created and will most likely proceed to be created within the future as a rapidly developing fabricating innovation. In arranging for recently made added substance manufacturing technologies to use the foremost suitable procedures with moved forward execution, it may be suitable to do a study of the subject concerning way arranging [8].

To utilize the manufacturing process to its fullest importance the manufacturing materials used must be of quality. Since these automated machines will be potentially used in various applications, for instance, in defense, aerospace engineering, disaster response, drones, education (lego, 3D printers, robot-teachers, etc.), exoskeletal robots, entertainment, humanoid, health-care robots, etc. The manufacturing of a quality robot involves the comparative analysis and application of suitable materials based on their different physical, chemical, or thermodynamic properties like weight, buoyancy (for underwater robots), resistance, temperature tolerance, tensile strength, etc. [9]. Some robotics developers may not give much attention to a robot's exterior, but the materials you select will affect its security, toughness, and even appearance. Any plan extension ought to take the movement of a robot, its ability to function near humans, the jobs it will carry out, and the environment into account. Future frameworks will incorporate cross-breed frameworks with human and automated administrators, metal and composite materials, added substance and subtractive fabricating strategies, and cyber and physical frameworks. Examining the associations between constituents and guidelines is so pivotal and important [9].

12.2.1 MATERIALS USED IN ROBOT DESIGNING

Following subsections describe the different materials' characteristics and availability in the field of robot designing [10] as described in Table 12.1.

TABLE 12.1 Materials Used in Robotics and Their Properties ⏎

S. No.	Material Name	Density (g/cm³)	Ductility	Tensile Strength (MPa)	Strength	Elasticity (GPa)	Cost (Rs. per gram)
1.	Aluminum	1.7	Highly ductile	90 (pure) 124 (alloy)	11 (MPa) (Pure) 400 (MPa) (Alloy)	70	2.833
2.	Kevlar	1.44	Highly ductile thermoplastic	70500	3620 (MPA)	130	2.799
3.	Carbon fibre	1.9	Highly ductile	4000	2500 (GPa)	500	1.802
4.	Graphene	2.27	Highly stretchable and ductile	125 GPa	42 N/m	1.15	4.096–122.80

12.2.1.1 STEEL

One of the materials that robot builders most as often as possible utilize is steel. On the off chance that you are making a robot that must withstand challenging situations, choosing this vigorous metal is shrewd. The steel can be solidified to between 100,000 and 300,000 pounds per square inch (psi) in different circumstances. To cement the steel, utilize a grouping with a tall carbon concentration. Customarily, steel is more suited to being made harder through warm drugs the more carbon it ought to. Set the steel, and utilize a collection with a tall carbon concentration.

Customarily, steel is more suited to being made harder through warm drugs the more carbon it has. Steel that withstands reiterated blows and ultra-wear-resistant steel are choices. Keep in mind that not with the proper hardware, as an example welding apparatuses, using this material can be challenging. Usually particularly genuine if you wish to form the steel to fit a certain dimension in order to overall design of the robot [11].

12.2.1.2 RUBBER

Commercial robots with adaptable outsides, such as human-like "skin," are getting to be increasingly well known. Additionally, cobots that collaborate with individuals advantage of having delicate surfaces. Elastic and adaptable polymers can accomplish that. A group of analysts from the College of Houston has reported an improvement in stretchy hardware which will act as fake skin, giving an automated hand the capacity to recognize between hot and cold conditions and giving benefits for an assortment of biomedical devices. The work is the primary semiconductor in elastic composite organize that empowers stretchability without any uncommon mechanical structure. Engineered skin is simply one utilized. Analysts anticipated that the improvement of delicate wearable hardware, such as well-being screens, restorative inserts, and human–machine interfacing, will be affected by the disclosure of a fabric that's delicate, bendable, stretchable, and twistable [12].

The gadgets were still utilitarian even after the analysts increased the elasticity by 50%. When designing robots, conventional semiconductors are troublesome to deal with since they are delicate, which is unfavorable for a robot that should twist. As a demonstration of their work, the analysts made an automated skin that can determine temperature after being immersed in a glass of water. To acknowledge the range of prospective employment for the degree, this was then modified to be able to recognize computer signals and interpret them into American Sign Language. Analysts from Stanford College and the National College of Singapore are moreover creating touch-sensitive polymer-skinned robots. Even though your robot's skin is made of elastic, its insides more often than not have difficult parts like CPUs and actuators.

However, a later endeavor involved making a delicate robot with a rubber-based computer. By and large talking, rubber-bodied robots are less unsafe than those built of harder materials. Also, they work well when taking care of sensitive merchandise like natural products. In pick-and-place exercises, Delicate Robotics' grippers adjust to such things without harming them. Robots are associated with guests at a few Disney topic parks, and there are plans to sometime in the not-so-distant future go past the glass-enclosed or remote-controlled animatronics to incorporate strolling robots all through the parks. It is basic to understand why elastic and plastic are beneficial for making exact robots that are too more secure to utilize around individuals [13].

12.2.1.3 ALUMINUM

Aluminum is less demanding to shape and lighter than steel but has a better cost point. Aluminum does not rust, in this way, it could be a great fabric on the off chance that you are concerned that a robot's outside would do so over time. Be that as it may, given that a few soggy circumstances can cause it to erode, you might think approximately coating the surface to avoid its potential erosion. The ability of aluminum to be cleaned to a bright luster makes it a commonly used material for robot exteriors. Aluminum not only provides the robot body's attractive appearance, but it also provides adequate durability [10].

Working with experts who provide three-way machines, which enable programming to meet the demands of double-sided preparation and aluminum cleaning technology, is another option. Many designers also used aluminum to protect the robot and its more delicate components. For example, Italian researchers created a robot strong enough to drag a 7200-pound fly down a runway. A roll cage made of aluminum housed the robot's parts, two computers, four electric engines, and four pressure-driven actuators.

12.2.1.4 KEVLAR

Kevlar may be an engineered texture broadly utilized to form bulletproof clothing. The main advantage is to take into account for robots outside due to a few of its attributes. It could be utilized as a covering for robots that need to be protected from extreme cold or heat. Kevlar does not dissolve or drip in hot environments, hence it may be a typical component of heat-resistant gloves. Kevlar neither corrupts in cold temperatures of −50°F nor does cryogenic conditions unfavorably influence the strands [11].

12.2.1.5 SEMICONDUCTORS

The mechanical autonomy (robotics) industry has been influenced by the semiconductor deficiency in a number of ways. Semiconductors are fundamental components of numerous robots, especially those that depend on progressed sensors and processors. Without these components, the generation and advancement of robots can be deferred or indeed stopped [14]. The semiconductor deficiency has caused a disturbance within the worldwide supply chain, which has influenced the accessibility and estimating of numerous basic components, counting microcontrollers, memory chips, and control administration gadgets. This has driven to expanded lead times, higher costs, and in a few cases, by and large shortage of certain components.

The effect of the semiconductor deficiency on the mechanical technology industry has been felt over the whole esteem chain, from producers to end-users. Mechanical autonomy producers have had to alter their generation plans, delay modern item dispatches, and in a few cases, decrease their general yield. End-users have experienced longer lead times for unused hardware, and in a few cases, have been constrained to pay higher costs for existing items [15].

By and large, the semiconductor deficiency has been a noteworthy challenge for the mechanical technology industry, but numerous companies are working to moderate the effect through vital sourcing, supply chain enhancement, and speculation in unused innovations.

12.2.2 MATERIALS FOR DESIGNING MAIN ROBOT COMPONENTS

Several types of robot technologies are shaping the world with their power, serving in healthcare, defense, education, textile, and more. The robotics sector is quite complex and can require much time to evolve to have solid growth as these technologies are influenced by the natural world, where solutions took millions of years to reach the highest level of perfection. An analysis of new technologies brings many trends in robotics which are followed by old technologies [16].

12.2.2.1 ARTIFICIAL MUSCLES AND ACTUATORS FROM CARBON NANOTUBES (CNT)

Carbon is considered as one of the most prevalent elements in the universe. Carbon allotropes having cylinder-like shapes are known as carbon nanotubes

(CNTs). Researchers used CNTs to build actuators and artificial muscles. CNT-based actuators have many capacity programs, including robotics, biomedical devices, and microelectromechanical structures. They are especially useful in applications where small, lightweight actuators are required, such as in area exploration or medical implants [17].

One of the key blessings of CNT-based actuators is their excessive energy density, which means they could keep a massive quantity of strength to a small extent. This makes them best for packages in which area and weight are at a top rate. But, there are nevertheless challenges that need to be addressed earlier than CNT-based total actuators may be broadly adopted. These include enhancing the reliability and sturdiness of the materials, in addition to locating approaches to manufacture them at scale. No matter those demanding situations, CNT-based artificial muscle tissue, and actuators can revolutionize a wide range of industries, from robotics and automation to aerospace and medicine [18]

12.2.2.2 ELASTIC ELECTRIC CABLE (EEC)

An elastic electric cable is a kind of cable that is designed to stretch maintaining its conductivity. It is an application that is commonly used where the cable needs to stretch such as in robotics and medical devices. These cables consist of conductive cables rounded by stretchable elastic material like an elastomer. These materials ensure the connection between wires while being stretched and deformed so that electrical current can flow without any interruption [18].

The key advantage of using these elastic electrical cables is their ability to withstand repeated stretching and deformation with conducting electricity throughout the wires. This makes them the ideal type to use in applications, where cables need to stretch and repeated bending like wearable tech and robotics limbs. The EEC can affect the electric properties of the cable, which will lead to signal degradation. And EEC may wear out which can impact durability and reliability. Despite those limitations, EEC still has a wide range of applications and important factors for more flexible electronic devices.

12.2.3 MOBILE AND STATIONARY ROBOTS IN AUTOMATION

As inventive mechanical autonomy producers proceed to provide different shape components, capabilities, and prices, the ever-increasing demands for robotics solutions are increasing the number of industries and applications. Nowadays there are six general categories grouped for robots. Table 12.2 gives a description about various available robots with their specific applications. This includes cylindrical robots, scara robots, polar robots, articulated robots, delta robots, cartesian robots, and collaborative robots [1, 4, 5]. Table 12.3 gives classification of mobile and stationary robots. The following subsection gives description about the principle of working used in designing of above mentioned robots [9].

TABLE 12.2 Types of Robot and Applications ⏎

Robots	Merits	Demerits	Applications
Cylindrical robots	Can carry more loads	Bulky	Automation of the welding process, application of assembly technology, and painting
Scara robots	Position consistency, compact footprint and simple mounting high speed with light loads	Suitable for light-to-medium-weight loads	Applications for high-speed, high-precision pick and place, such as engraving and material handling
Polar robots	good capacity for lifting loads	Large size, intricate design, and high cost	Welding, material handling, and injection molding
Articulated robots	Good adaptability and rapidity	Complex and pricey	Painting, coating, welding, and packaging call for working with circular symmetry.
Delta robots	Rapidity and acceleration	Unable to carry large weights	Packaging and soldering applications for rapid pick and place
Cartesian robots	Simpler designs and easily operatable, Fast and efficient	Bulky, Poor acceleration, Less flexible	Plotting, 3D printing, linear pick and place, and cutting
Collaborative robots	Human-friendly, adaptable, user-friendly, and flexible	Slow, pricey, large, and needed many approvals	Variety of tasks such as picking up bins, screwing, polishing, and sealing.

TABLE 12.3 Most Known Robots in Mobile and Stationary Sector ⏎

Mobile	Stationary
• AMRs	• Articulated robots
• AGVs	• Cobots
• Humanoids	
• Hybrids	

12.2.3.1 AUTONOMOUS MOBILE ROBOTS (AMRs)

AMRs make decisions in real time as they go and move throughout the world. These are mobile solutions that require the least human guidance or input to complete their task. To create an educated decision—whether that is moving to maintain a strategic distance from an oncoming laborer, accurately picking the proper allocate, or selecting a fitting surface to clean The on-board processing equipment helps them analyze it. To get information about surrounding technologies such as cameras and sensors are used [19].

12.2.3.2 AUTOMATED GUIDED VEHICLES (AGVs)

AVGs rely on the predefined path or tracks and require operators' sight while AMRs traverse environments freely. These are usually used to move items in controlled environments such as factory floors or warehouses. Simply used for delivering materials to their designated place. Number of technologies, such as floor-surface-mounted appealing tape or bars, lasers, magnet/gyroscope-based inertial direction, and optical sensors, provide guidance for the vehicles as they explore the location [20].

12.2.3.3 ARTICULATED ROBOTS

To emulate the functions of human arms, articulated robots (moreover known as automated arms) are implied. From two to ten rotary joints, these can feature anywhere. A more noteworthy degree of motion-making these perfect for circular segment welding machines, bundling, fabric taking care of, and machine tending are permitted by extra joint or pivot [20].

12.2.3.4 HUMANOIDS

Maybe some mobile humanoid robots technically are said to be the space of an AMR, this phrasing is utilized to recognize those robots that perform human-centric capacities and regularly carry on human-like [17]. From acting as they carry out tasks such as giving headings or offering concierge administrations, sense, and arrange, humanoids utilize numerous innovation components such as AMRs [4].

12.2.3.5 COBOTS

These robots are designed to work with humans. While other robots do their task on their own, or in disconnected work environments, cobots can share spaces with people or laborers to assist them to extemporize and accomplish more. During day-to-day workflows, cobots are usually used to eliminate strenuous, manual, or dangerous tasks. Some cobots can operate by learning from human movements and by responding to them. Technologies that guarantee the security, consistency, and security of the arrangement, besides equipment plan, sensors, and actuators, proficient data handling, video preparing, arranging, and numerous areas from counterfeit insights scenes [5].

12.2.3.6 HYBRIDS

A hybrid type of robot is made by combining various types of robots that can perform more complex tasks than other robots. For example, to handle packages in a warehouse, the robotic arm is combined with AMR. Also, more functionality is fitted into the particular solution (robot), and its computing capabilities are consolidated. Most hybrid types of robots use wheel-leg mechanisms as locomotion systems [21].

12.3 TRENDS IN ROBOTICS TECHNOLOGY

The past two decades have seen critical progressions in mechanical technology innovation, driving to the advancement of more modern and competent robots in different businesses. Figure 12.1 gives description about top users of robots by industries such as automotive, electrical and electronics, plastic and chemicals, metal products, etc. Figure 12.2 provides service robots deployment of three years 2019–2021, where it has been observed that compound annual growth rate from 2020 to 2023, gives details about sales of mobile autonomous robots using in logistics are projected to grow by 31% annually. Also, the International Federation of Robotics (IFR) forecasts a 40% annual growth in sales of mobile robots that are designed for public usage [22]. AI has made critical strides over the past 20 years, leading to the development of smarter and versatile robots. AI permits robots to memorize from their environment, make choices based on information inputs, and adjust to changing circumstances.

As explained in Section 12.1, Cobots have ended up progressively prevalent within the final decade, outlined to work nearby people in fabricating,

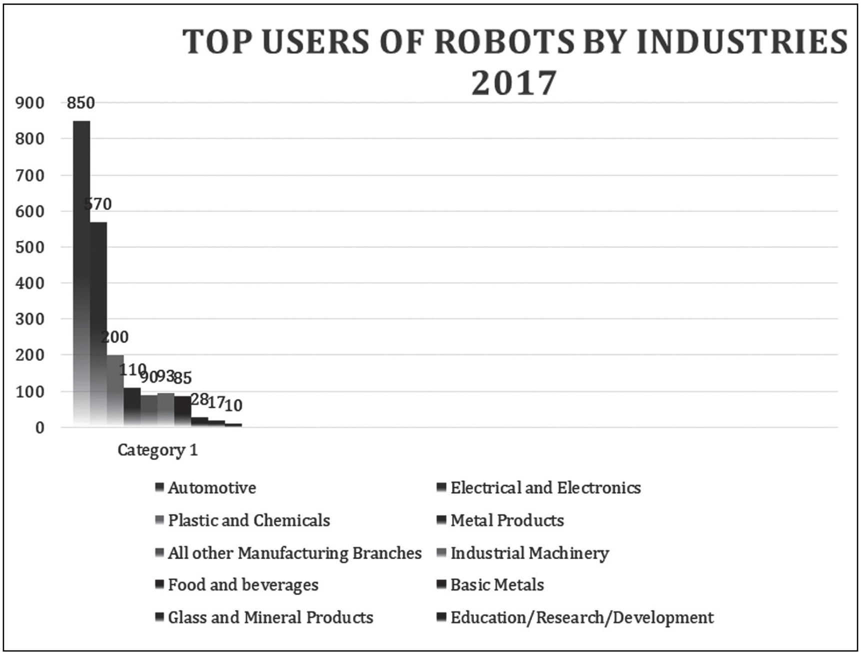

FIGURE 12.1 Robotic technology top users in industries in 2017. ⏎

Source: Modified from Ref. [22].

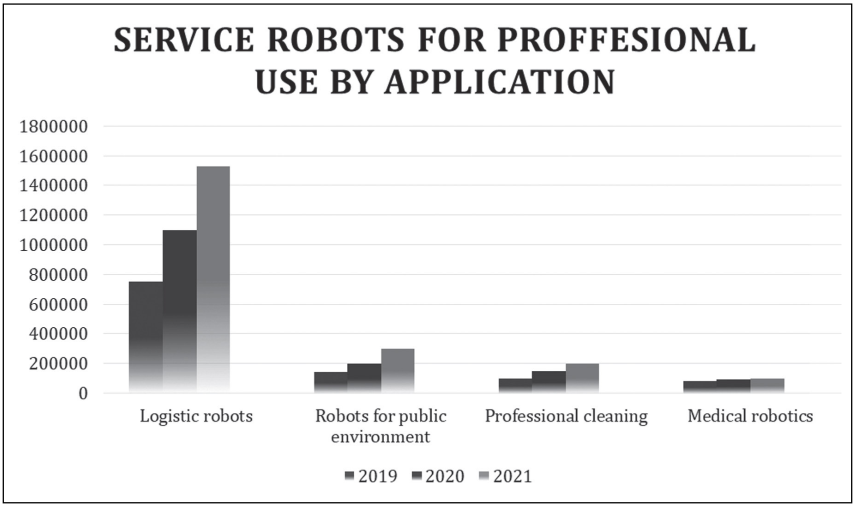

FIGURE 12.2 Service robots deployment where *X*-axis represents fields of robotics and *Y* represents the number of '000 of units. ⏎

Source: Modified from Ref. [24].

healthcare, and other businesses. These robots are modified to be secure and can perform assignments that are monotonous, unsafe, or require exactness. Other types of robots are independent robots, which are more common in fabricating, coordination, and other businesses. These robots can work without human intercession and make choices based on data inputs and natural conditions.

Portable robots have ended up progressively modern within the past 20 a long time, with applications extending from distribution centre robotization to independent vehicles. These robots can explore complex situations and perform a assortment of errands, counting transportation and assessment. Delicate mechanical autonomy includes the utilize of adaptable and deformable materials to make robots that can adjust to their environment and perform sensitive errands. This innovation has applications in fields such as healthcare, fabricating, and space investigation [14].

Exoskeletons are wearable robots that expand human quality and portability. These gadgets have applications in areas such as healthcare, manufacturing, and defense. Drones have ended up progressively well known within the final two decades, with applications extending from airborne photography to bundle conveyance. They are too utilized in agribusiness and natural observing [17, 18].

3D printing has revolutionized the way that robots are planned and built. It permits for more complex and customized plans, as well as quicker and cheaper generation. Swarm mechanical technology: Swarm robotics includes the coordination of huge bunches of robots to perform assignments collectively. This innovation has applications in areas such as look and protect, farming, and development [16].

Hence, this field has seen noteworthy headways in robotics innovation, with new applications and capabilities rising in different businesses. These headways have been driven by progress in AI, materials science, and manufacturing innovation. It is likely that this slant will proceed within the future, leading to indeed more modern and able robots. As mechanical technology innovation proceeds to advance, it has the potential to convert businesses and make strides people's lives in modern and imaginative ways [23].

12.4 METHODOLOGY

As of now, lightweight is one of the most common concerns within the car industry concerning vitality proficiency. The emanation of gasses and the fuel effectiveness of vehicles are two basic issues. By diminishing the weight of Hexapod parts, fuel productivity can be made strides. Inquire about and advancement play a noteworthy part in lightweight materials for diminishing taking a toll, and expanding their capacity. To be reused, empowering their integration into vehicles, and maximizing their fuel economy adequacy. There emerges a requirement for creating a novel era of materials that will combine both weight decrease and security issues. Carbon fiber-reinforced plastic offers the taking-after benefits [20]. Realizing lightweight concepts with the finest conceivable lightweight potential. Carbon fiber composite plastic has extraordinary particular solidness, particular strength, and weakness properties compared to commonly utilized metals. The points of interest of carbon fiber-reinforced plastic within the car industry incorporate weight diminishment, portion integration and lessening, crashworthiness, strength, sturdiness, and stylish request. Carbon fiber-strengthened plastic is an amazingly flexible fabric. It has been utilized broadly in different applications such as the aviation industry, sports hardware, the oil and gas industry, and the car industry. Keeping in see the previously mentioned focal points of carbon fiber composite plastic, the creators have displayed a brief audit of carbon fiber for car and industrial applications [17, 25].

Figure 12.3 explains about the general functioning of robots which includes mainly following units like controller, actuators, sensors, etc. First, robot has been given a task and the designed robot model which may include microcontroller programmed for the required task. The controller, such as robotic hand, receives the information from the robot model which is used to activate the actuators. Here sensors serve as the input unit and actuators are for giving final output like hand movement for the given task.

The plan of the hexapod robot is started by planning diverse parts on a program like Blender and AutoCAD. We are using Blender for different animations and product details and AutoCAD for calculations and designing other hexapod parts like the Chassis (Robot body and bolster), Robot leg, Robot arm, Engine Base, Engine back, crankshaft, settled shaft, engine shaft, and at long last the get together of the robot. We are using graphene for most of the parts of the hexapod. For less vulnerability, we are designing it as a drone system. In total, we are going to use four motors for the movement of the hexapod. The hexapod is comprised six straight ball-screw actuators driven by six DC engines. We are using Arduino UNO to manually control the movement of the hexapod. We are using 12 micro servos (MG90S) with metal gears for high torque with less weight. An HC-SR04 Ultrasonic ranging module is used for the detection of obstacles coming in between the path of the hexapod. 60 M3 bolts +120 nuts and washers are used for fitting and fixing the joints. A battery of NiMH or Li-ion will be used for the source. Moreover, finally a multimeter soldering iron and drill will be used [19, 26].

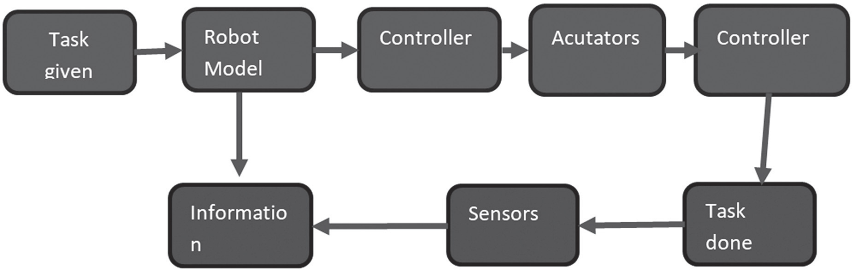

FIGURE 12.3 Functioning block diagram of robot ⏎

12.4.1 MATERIALS USED

Hexapods are a sort of robot that has six legs, permitting them to move in complex and uneven territory with deftness and exactness. These robots have ended up progressively prevalent in later a long time due to their flexibility and progressed control capabilities. In this chapter, we are going to investigate the mechanics and science behind hexapod robots, counting their kinematics and walk designs [27, 28].

Graphene: It is a strong and lightweight metal whose quality primarily comes from the solid covalent bonds of the carbon particles. It will help hexapod in his strength, and toughness, and will decrease his weight which will help in flying for a longer duration [12].

Drone System: Unmanned aerial vehicles (UAVs) or unmanned airship frameworks are more formal names for drones [28]. A drone is a type of flying robot that can be remotely controlled or can fly on its own using flight plans that are controlled by software and on-board sensors and a global positioning system.

Motors: A motor is only an electromechanical device that converts electrical energy into mechanical energy. And this mechanical energy will help the hexapod to move and fly.

MG90S: It is a micro servo motor with metal equipment. This tiny, lightweight servo has a tall yield control, making it ideal for RC airplanes, quadcopters, or Mechanical Arms.

HC-SR04: The HC-SR04 is a reasonable, easy-to-use ultrasonic remove sensor, with 2 to 400 cm. It is commonly utilized in obstacle-avoiding robots and mechanization ventures.

Battery: This is a device made up of one or more cells that convert chemical energy into electrical energy for use as a source of electricity. Using 4.8–6-V battery.

Blender: It is a 3D creation suite that is open-source and free. It supports the entire 3D workflow, including modeling, fixing, movement, recreation, rendering, compositing, movement tracking, and even video editing and entertainment production.

AutoCAD: AutoCAD is a computer-aided plan program that allows to more quickly and efficiently than by hand, draw, and edit complex 2D and 3D plans.

12.4.2 FLYING HEXAPOD MATHEMATICAL MODEL

Based on the Newton–Euler equation and driven by the physical characteristics described in the part before, this section gives a mathematical model of a hexapodopter in flight. The position vector r = x^T, y^T, z^T and the three Euler angles $q = [\phi, \theta, \psi]$ indicate where B is in relation to W and how it is oriented. Rigid body dynamics can be broken down into two components [15, 18]. Translation and rotation, respectively, are represented in Equations 12.1 and 12.2.

$$m\ddot{r} = R(q)F - mg - \dot{q} \times m\dot{r} \tag{12.1}$$

$$I\ddot{q} = \tau - \dot{q} \times I\dot{q} \tag{12.2}$$

with m being the total mass of the rigid body, I being its inertial network, g being the acceleration due to gravity, $R(q)$ being the revolution matrix, F being the entire constraint, and T being the overall torque applied to the rigid body. We use the formulas $f = k\_f\, w2$ and $i = (1)\ i\_(k\_T)\ w2$ to calculate the relationship between the engine's precise speed i and the pushing drive it generates [29]. And "(−1)" characterizes the sign that demands that the propeller's revolution sense be taken into account. From this, each engine applies a drive and torque determined with respect to the body outline are shown in Equations 12.3 and 12.4:

$$f_i = k_f w_i^2\ \hat{n}_i \tag{12.3}$$

$$\tau_i = (k_f\ {}^\wedge P, it_B \times \hat{n}_i + (-1) i_{k_T} \hat{n}_i)\omega_i^2 \tag{12.4}$$

where coaxial unitary vector with the Z_p is $\hat{n}_i$, i is motor axis, f_i is force and τ_i is torque, groupable into a wrench w_i . $f_i = k_f\, w_i^2$ represents the thrust force magnitude and motor i has T_i as transfer colon vector. As a result, it is possible to determine the total force and torque applied to the six thrust motors with regard to B [30]. Using the transfer matrix T, the dynamics of the Hexapodopter can be rewritten as follows in Equations 12.5 and 12.6, respectively:

$$m\ddot{r} = R(q)T_f\,\Omega - mg - m\dot{q}\times\dot{r} \tag{12.5}$$

$$I\ddot{q} = T_\tau\,\Omega - \dot{q}\times I\dot{q} \tag{12.6}$$

12.4.3 HOLONOMIC ANALYSIS

On the off chance that the hexapodopter may be a 6 DoF vehicle *T* should rise to the rank of 6, but that is typically insufficient. We used the force-closure idea to show and validate that the hexapodopter might be a holonomic UAV. Force-closure in A become familiar with rhypothesis A mechanical hand has been shown to be able to control a protest while maintaining translational and rotational harmony using force-closure [30].

We used this concept to demonstrate that the six pushing powers that control the Hexapodopter's body while it is in flight can measure the strengths and torques produced by any unpleasant outside force. A drive acting on a protest on a contact point Ci is modeled by a four-component vector $fi = [f_n, f_o, f_t, f_m]_i^T$ to help with the hypothesis, where the component f_n is the ordinary component, f_o and f_t are the two opposite digression components, and f_m speaks to the turn minute almost the contact ordinary. The applied torque by a drive fi on a unbending body is modeled with a get a handle on network Gi ∈ $R^{6\times4}$ and the resultant torque can be computed as $w_i = G_i f_i$, where G_i is characterized by [14] in Equation 12.7 as follows:

$$G_i = [\hat{n}\,\hat{o}\,\hat{t}\; r\times\hat{n}\; r\times\hat{o}\; r\times\hat{t}\; 0\,\hat{t}]_i \tag{12.7}$$

where $\hat{n}_i$ is the normal vector to the unbendable body's surface at the contact point C_i while $\hat{o}_i$ and $\hat{t}_i$ are inverse diversion of the orthonormal layout by directing vectors to the surface contact point C_i. Within the occasion that J powers are connected in inflexible design which are going to be tested the adjust position of resolute body by calculating and foreseeing the outcome torque p to break to zero. At that point, this agreement condition is $p = G_n$ f, where G_n matrix is represented by the following Equations 12.8 and 12.9:

$$G_n = [G_1\; G_2 \ldots\ldots\ldots G_J] \in \mathrm{R}^{6\times4J} \tag{12.8}$$

$$f = \left[f_1^T f_2^T \ldots\ldots\ldots\ldots f_J^T\right] \in R^{4JX1} \tag{12.9}$$

12.5 RESULTS AND DISCUSSION

Robots are also making an effect within the development industry. They can be utilized to exhume and move overwhelming materials, lessening the requirement for manual labor. Robots can moreover be utilized to examine buildings and bridges for abandons, decreasing the hazard of mishaps and making strides in security.

Robots have made critical commitments to numerous businesses. They have moved forward in proficiency, precision, and security whereas lessening costs and labor. As innovation proceeds to progress, robots will likely be gotten to be indeed more predominant in completely different businesses, changing the way we work and live [1, 2].

Robots have revolutionized the way we live and work. With their progressed capabilities and flexibility, robots are progressively being utilized in different businesses, from fabricating and horticulture to healthcare and investigation. One of the foremost interesting sorts of robots is the hexapod robot, which may be a six-legged robot that can move in any direction, climb over deterrents, and navigate the unpleasant territory. In this chapter, we have explored about the applications of different types of robots including the hexapod robot and the material used for designing was also discussed.

Automated innovations have progressed essentially in later a long time, and have applications in a wide extend of businesses, from healthcare and fabricating to space investigation and defense. Here, we will talk about a few of the later progresses and applications of automated advances. One major range of advancement in automated advances is within the improvement of humanoid robots. These robots are planned to imitate human developments and have the capacity to associate with people in a characteristic way. For case, Sophia, a humanoid robot created by Hanson Mechanical technology, has the capacity to recognize human faces and expressions and react in a way that imitates human behavior [27].

Another zone of progression is within the improvement of collaborative robots or cobots [11], which work nearby people to improve efficiency and proficiency. These robots are outlined to be secure to work nearby people and can perform errands such as gathering parts or taking care of materials. Automated advances have moreover made noteworthy commitments to the healthcare industry, with the advancement of surgical robots that can perform negligibly intrusive surgeries with more noteworthy precision and accuracy. Furthermore, robots are being created to help with errands such as physical treatment and senior care.

Within the fabricating industry, mechanical advances have been broadly received for assignments such as gathering, review, and bundling. These robots are able to work at a quicker rate and with more prominent exactness than human laborers, driving to expanded proficiency and efficiency. The improvement of autonomous robots has moreover opened up unused conceivable outcomes for space exploration and defense. For example, the Mars Wanderer could be a mechanical vehicle that's able to investigate the Martian surface and transmit information back to Soil. Independent rambles are moreover being created for extend of applications, counting observation and delivery administrations [6].

In any case, there are moreover concerns approximately the effect of automated innovations on business and the economy. As robots become more progressed and competent of performing assignments that were already done by people, there is a chance of work relocation and a broadening wage hole. Overall mechanical innovations have made critical progresses in later a long time and have applications in a wide extend of businesses. While there are concerns regarding how it might impact business and the economy, further research and development will probably result in more advanced and capable robots with more notable potential uses.

12.6 CONCLUSION

Automated innovation has come a long way in later a long time, and there are presently different sorts of robots that serve diverse purposes. These robots are planned to perform assignments that are troublesome or outlandish for people to do, or to mechanize monotonous assignments, making them more productive and cost-effective. A few of the sorts of robots incorporate mechanical robots, benefit robots, restorative robots, and military robots. Mechanical robots are utilized in fabricating and getting together lines to progress generation and quality. These robots are modified to perform monotonous errands such as welding, portray, and pick-and-place operations. They are too utilized in perilous situations where human laborers may be at chance.

Benefit robots, on the other hand, are planned to connect with people in a assortment of settings. These robots can be utilized in healthcare, neighborliness, retail, and other businesses to perform errands such as cleaning, cooking, and giving clients benefits. They can moreover be utilized in homes to help with errands such as vacuuming and grass care. Therapeutic robots have been created to move forward persistent results and diminish healthcare costs. These robots can be utilized for assignments such as surgery, conclusion, and recovery. They can also be utilized in inaccessible areas to supply therapeutic care to patients who are incapable to visit a specialist in individual.

Military robots are utilized for a assortment of assignments, counting observation, observation, and bomb disposal. They are outlined to function in unsafe situations, such as war zones, where human officers may be at hazard. These robots can also be utilized in search-and-rescue missions to find survivors in fiasco zones. Moreover, automated innovation is getting to be progressively common in different industries, and this slant is anticipated to proceed within the coming a long time. As innovation propels, robots are getting to be more advanced and flexible, and their potential employments are for all intents and purposes boundless. From manufacturing and healthcare to farming and space investigation, robots are balanced to convert numerous zones of our lives and bring approximately noteworthy changes in proficiency, safety, and efficiency.

In any case, there are too many concerns approximately the effect of robots on human work, and a few contend that the expanding utilize of robots may lead to work misfortune and disparity. It is critical to address these concerns and guarantee that the benefits of automated innovation are shared by all individuals of society. Overall the use of mechanical innovation may bring around a few challenges, its potential benefits are critical. By grasping and utilizing these innovations, we are able make a more secure, more efficient, and more beneficial world for all.

KEYWORDS

- **materials for robot manufacturing**
- **hexapod**
- **robotic technology**
- **automation**
- **holonomic analysis**

REFERENCES

1. Pagliarini, L., Lund, H. The future of robotics technology. *Proc. Int. Conf. Artif. Life Robot.*, **2017**, *22*, 29–32. https://doi.org/10.5954/ICAROB.2017.IS-1.
2. Lin, P., Abney, K., Bekey, G.A. *Robot ethics: the ethical and social implications of robotics*. MIT Press, 2011.
3. Diodato, M.D., Damiano, R.J. Robotic cardiac surgery: overview. *Surg. Clin.*, **2003**, *83*(6), 1351–1367. https://doi.org/10.1016/S0039-6109(03)00166-X.
4. Kajita, S., Hirukawa, H., Harada, K., Yokoi, K. *Introduction to humanoid robotics*; *Springer tracts in advanced robotics*; Springer: Berlin, Heidelberg, 2014, Vol. 101. https://doi.org/10.1007/978-3-642-54536-8.

5. Kernbach, S. *Handbook of collective robotics: fundamentals and challenges*, CRC Press, 2013.
6. Zammuto, R.F., O'connor, E.J. Gaining advanced manufacturing technologies' benefits: the roles of organization design and culture. In *Organizational innovation*, Routledge, 1998.
7. Bhatt, P.M., Malhan, R.K., Shembekar, A.V., Yoon, Y.J., Gupta, S.K. Expanding capabilities of additive manufacturing through use of robotics technologies: a survey. *Additive Manuf.*, **2020**, *31*, 100933. https://doi.org/10.1016/j.addma.2019.100933.
8. Li, K., Zhang, J., Wang, L., Zhang, M., Li, J., Bao, S. A review of the key technologies for SEMG-Based human-robot interaction systems. *Biomed. Signal Process. Control*, **2020**, *62*, 102074. https://doi.org/10.1016/j.bspc.2020.102074.
9. Radha, H.M., Hassan, A.K.A. A survey on bio-signal analysis for human-robot interaction. *Int. J. Electr. Comput. Eng.*, **2022**, *12*(6), 5998.
10. Correll, N., Rus, D. Architectures and control of networked robotic systems. In *Handbook of collective robotics*. Jenny Stanford Publishing, 2013, p. 24.
11. Safeea, M., Bearee, R., Neto, P. An integrated framework for collaborative robot-assisted additive manufacturing. *J. Manuf. Process.*, **2022**, *81*, 406–413. https://doi.org/10.1016/j.jmapro.2022.06.067.
12. Yu, W., Sisi, L., Haiyan, Y., Jie, L. Progress in the functional modification of graphene/ graphene oxide: a review. *RSC Adv.*, **2020**, *10*(26), 15328–15345. https://doi.org/10.1039/D0RA01068E.
13. Pathak, R., Shende, P., Mahabal, C. Swarm robotics fundamentals and applications. *IJIERT*, **2016**, 1–4.
14. Arena, P., Patanè, L., Taffara, S. Energy efficiency of a quadruped robot with neuro-inspired control in complex environments. *Energies*, **2021**, *14*(2), 433. https://doi.org/10.3390/en14020433.
15. Quinn, R.D., Offi, J.T., Kingsley, D.A., Ritzmann, R.E. Improved mobility through abstracted biological principles. In *IEEE/RSJ International Conference on Intelligent Robots and Systems*, 2002, Vol. 3, pp. 2652–2657. https://doi.org/10.1109/IRDS.2002.1041670.
16. Rothemund, P., Kim, Y., Heisser, R.H., Zhao, X., Shepherd, R.F., Keplinger, C. Shaping the future of robotics through materials innovation. *Nat. Mater.*, **2021**, *20*(12), 1582–1587. https://doi.org/10.1038/s41563-021-01158-1.
17. Boxerbaum, A.S., Oro, J., Peterson, G., Quinn, R.D. The latest generation Whegs™ robot features a passive-compliant body joint. In *2008 IEEE/RSJ International Conference on Intelligent Robots and Systems*, 2008, pp. 1636–1641. https://doi.org/10.1109/IROS.2008.4650997.
18. Allen, T.J., Quinn, R.D., Bachmann, R.J., Ritzmann, R.E. Abstracted biological principles applied with reduced actuation improve mobility of legged vehicles. In *Proceedings 2003 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS 2003) (Cat. No.03CH37453)*, 2003, Vol. 2, pp. 1370–1375. https://doi.org/10.1109/IROS.2003.1248835.
19. Tan, H., Zhang, H., Wang, Y., Huang, Z., Li, L., Chen, X., Huang, T., Chen, X., Chen, S. Dynamics modeling and gait analysis of transport-oriented hexapod robot. In *Advances in guidance, navigation and control*, Yan, L., Duan, H., Yu, X., (Eds.), Lecture Notes in Electrical Engineering, Springer: Singapore, 2022, pp. 4337–4350. https://doi.org/10.1007/978-981-15-8155-7_360.

20. Saranli, U., Buehler, M., Koditschek, D.E. RHex: a simple and highly mobile hexapod robot. *Int. J. Rob. Res.*, **2001**, *20*(7), 616–631. https://doi.org/10.1177/02783640122067570.
21. Eich, M., Grimminger, F., Kirchner, F. Proprioceptive control of a hybrid legged-wheeled robot. In *2008 IEEE International Conference on Robotics and Biomimetics*, 2009, pp. 774–779. https://doi.org/10.1109/ROBIO.2009.4913098.
22. Which countries and industries use the most robots? https://www.stlouisfed.org/on-the-economy/2019/november/robots-affecting-local-labor-markets (accessed Apr 15, 2023).
23. Leng, X., Piao, S., Chang, L., He, Z., Zhu, Z. Dynamic running hexapod robot based on high-performance computing. *J. Supercomput.*, **2020**, *76*(2), 844–857. https://doi.org/10.1007/s11227-019-02988-2.
24. Borgne, M.L. Service robotics: definition and market growth [Online] [(Cited: 15 Apr. 2023]. https://awabot.com/en/service-robotics/.
25. Li, M., He, Z., Zha, F. Design and analysis of a semi-circular flexible hexapod robot MiniRHex. In *2018 13th World Congress on Intelligent Control and Automation (WCICA)*, 2018, pp. 418–423. https://doi.org/10.1109/WCICA.2018.8630613.
26. Rafeeq, M., Toha, S.F., Ahmad, S., Razib, M.A. Locomotion strategies for amphibious Robots-A review. *IEEE Access*, **2021**, *9*, 26323–26342. https://doi.org/10.1109/ACCESS.2021.3057406.
27. A roadmap to industry 4.0: smart production, sharp business and sustainable development. *Advances in science, technology & innovation*, Nayyar, A., Kumar, A., (Eds.), Springer International Publishing: Cham, 2020. https://doi.org/10.1007/978-3-030-14544-6.
28. Tomić, T. Evaluation of acceleration-based disturbance observation for multicopter control. In *2014 European Control Conference (ECC)*, 2014, pp. 2937–2944. https://doi.org/10.1109/ECC.2014.6862237.
29. Wang, H., Fan, Y., Fang, B., Dai, S. Generalized linear discriminant analysis based on euclidean norm for gait recognition. *Int. J. Mach. Learn. & Cyber.*, **2018**, *9*(4), 569–576. https://doi.org/10.1007/s13042-016-0540-0.
30. Soto-Guerrero, D., Ramírez Torres, J.G. The hexapodopter: a holonomic flying hexapod. In *2017 14th International Conference on Electrical Engineering, Computing Science and Automatic Control (CCE)*, 2017, pp. 1–6. https://doi.org/10.1109/ICEEE.2017.8108873.

CHAPTER 13

ROLE OF SMART MATERIALS IN THE ADAPTATION OF ELECTRIC VEHICLES

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ABSTRACT

This chapter explores the role of smart materials (SMs) in the adaptation of electric vehicles (EVs). With the global push toward sustainable transportation, the demand for EVs has increased at full tilt. However, one of the main challenges facing the preponderate adoption of EVs is their long charging periods and limited running range. SMs have a strong potential to address these challenges by give the green light to the development of more reliable and efficient EV components, such as batteries, motors, and energy storage systems. This chapter provides an overview of the present state of SMs along with their potential applications in the development of EVs. It also discusses the advantages and limitations of different kinds of SMs and highlights a few of the most promising research in the field. Finally, the chapter concludes with a discussion of the future prospects for SMs in the adaptation of EVs and their potential impact on the transportation industry.

13.1 INTRODUCTION

Smart materials (SMs) have revolutionized various industries, and the automotive industry is no exception. Electric vehicles (EVs) are gaining popularity as a sustainable transportation option, and SMs are playing a crucial role in their adoption. SMs are those materials that can respond, sense, and adapt to environmental stimuli. They have some unique qualities that make it ideal for use in EVs, where efficiency, safety, and sustainability are paramount [1].

The transition to EVs is essential for reducing carbon footprints and lightening the effects of rapid climate change. However, EVs face challenges such as long charging times, limited range, and high production costs. SMs offer solutions to these challenges by improving vehicle efficiency, enhancing safety, and reducing the overall cost of production. They can also increase the sustainability of EVs by diluting the environmental effect of their manufacturing as well as operation [2].

This chapter explores the role of some SMs in the adoption of EVs. It begins by discussing the need for SMs for EV and the possible types of SMs used in their production. It then delves into the advantages of adopting SMs, including improved vehicle efficiency, enhanced safety, and increased sustainability. The chapter also discusses the challenges and limitations of using SMs in EVs and the future directions for their development and implementation. Overall, this chapter highlights the promising walk-on part of SMs in the widespread adoption of EVs and the transition to a sustainable transportation system [3].

13.2 THE NEED OF SM IN EVS

EVs are now becoming progressively popular as people strive to reduce its carbon footprint and adopt more sustainable modes of transportation. However, there are still some challenges to be overcome in order to make EVs more efficient, affordable, and practical. One of the key solutions lies in the area of research development of these materials.

SMs are materials which could change their behavior for reply to external stimuli, like heat, electricity, etc. These materials have power to revolutionize lots of industries, including automotive manufacturing. SMs can be used to make EVs lighter, more efficient, and safer.

Out of the literature, the most promising use of these materials in EVs is the development of high-strength and lightweight materials. The weight of a vehicle has a significant impact on its efficiency, and therefore, its range. By using lightweight materials, such as carbon fiber-reinforced polymers (CFRPs), EVs can become more energy efficient, allowing them to travel further on a single charge. However, lightweight materials can also compromise the strength and durability of the vehicle. SMs can help overcome this challenge by providing a combination of lightweight and high-strength properties. For example, researchers are working on developing materials that can switch from a soft and flexible state to a hard and rigid state to respond to different conditions [4–5].

SMs can also improve the safety of EVs. For example, researchers are developing stuff which can feel changes in temperature or pressure and respond accordingly. These materials can be used to detect and prevent overheating, which is a common problem in EVs. SMs can also be used to make EVs more crash-resistant by providing a combination of strength and flexibility.

In summation to these applications, SMs can be applied to enhance net efficiency of EVs due to reducing energy losses. For example, researchers are developing materials that can convert waste heat into electricity, which can then be used to power the vehicle. This could significantly improve the efficiency of EVs, allowing them to travel further on a single charge.

As the world transitions toward cleaner and more sustainable energy sources, EVs are gaining significant momentum as an alternative to traditional gasoline-powered cars. However, with this shift comes the need for more efficient and reliable components to power these vehicles. This is where SMs come into play, offering a promising solution for the challenges facing the EV industry [6–7].

These materials have the capacity to revolutionize the line EVs are built as well as operated, making e-vehicle more efficient, safer, and environmental friendly.

The main challenges opposing the EV sector is the limited range of EVs due to the limitations of current battery technology. SMs can help to enhance the range of e-vehicles by improving the efficiency of battery management systems and energy storage systems. For example, SMs like graphene can enhance the conductivity of the electrode materials in batteries, resulting in faster charging time and longer battery life.

Another major challenge for EVs is the weight of the vehicle, which can affect the overall performance and efficiency. SMs can help minimize the weight of EVs by replacing heavy traditional materials with lightweight and strong alternatives. For instance, CFRP composites can replace steel in the body of the vehicle, resulting in a lighter and more aerodynamic design.

Furthermore, SMs can increase the safety of EVs by offering better self-healing capabilities and crash resistance. For instance, shape-memory alloys (SMAs) can be taken in the body of the vehicle to absorb the energy of a collision and recover their original shape afterward. This can help minimize the chance of injury to passengers and increase the lifespan of the vehicle.

In addition to the benefits for EVs themselves, SMs can also have a positive impact on the environment. For example, materials like thermoelectric generators can convert waste heat from the vehicle's engine into usable electricity, reducing the overall energy consumption and carbon emissions.

Overall, the application of SMs in EVs is crucial for the development and growth of the industry. These materials can help address the challenges facing the EV market, including limited range, weight, safety, and environmental impact. As the demand for EVs continues to grow, SMs will play a key role in making EVs more efficient, reliable, and sustainable.

EVs are gaining popularity as they offer a clean and efficient mode of transportation. They are powered by batteries that convert electrical form of energy into mechanical form of energy to provide a driven form to EVs. However, the current generation of EVs still face several challenges such as low range, slow charging, and high cost. SMs can offer a promising role in addressing these challenges and making EVs more efficient and affordable.

They have the ability to sense, actuate, and control their vicinity, making them best for application in various purposes, including EVs. Following are some ways SMs can enhance EVs [8].

13.2.1 ENERGY HARVESTING

EVs rely on batteries for power, and one of the challenges is limited driving range. However, SMs can help in energy harvesting, where they can convert wasted energy into usable electrical energy. For example, piezoelectric materials can convert vibrations from the vehicle's movement into electrical energy, which can then be stored in the battery. This technology can help extend the driving range of EVs by making them more energy-efficient [9].

13.2.2 LIGHTWEIGHTING

Another challenge for EVs is their weight, which affects their efficiency and driving range. SMs like SMAs and composites can help reduce the weight of EVs. SMAs have the property to change their shape in response to heat or stress, which can be used to make lightweight components such as springs or shock absorbers. One another way is composites, which are formed by combination of two or more materials to create a most competent material that is stronger and lighter than the individual materials. These materials can help make EVs more efficient and reduce their carbon footprint.

13.2.3 THERMAL MANAGEMENT

EVs generate a lot of heat, especially during charging and driving. SMs such as thermoelectric materials can be used for thermal management, where such material can convert waste thermal energy into cooling or electricity. This technology can help improve the efficiency of EVs and reduce their dependence on air conditioning systems, which can drain the battery.

13.2.4 SELF-HEALING

EVs face wear and tear, which can lead to damage and reduce their lifespan. SMs such as self-healing polymers can help address this issue by repairing themselves when damaged. These materials can help reduce maintenance costs and extend the lifespan of EVs.

EVs are now proven more popular because of numerous benefits over traditional combustion engine vehicles. EVs offer a cleaner and more sustainable mode of transportation, dependence on conventional fossil fuels and reducing carbon footprint. However, the development of EVs has brought about a new challenge: the need for SMs.

For example, researchers have developed SMs that can help prevent the degradation of the battery. These materials can sense the charging condition of the battery and adjust the charging rate accordingly, reducing the likelihood of overcharging or undercharging. This practice can help to increase the life of the battery and minimize the count of frequent replacements.

Another potential utilization of SMs in EVs is in the development of self-healing materials. These materials can repair automatically when impairment, reducing the chance for repairs and replacements. This can help minimize the environmental impact of large scale manufacturing and disposing of goods.

EVs are subject to wear and tear, and even minor damage can compromise the vehicle's performance and safety. Self-healing materials can help overcome this challenge by repairing minor damage automatically. For example, researchers are working on developing materials that can heal small cracks and scratches using heat or light.

13.3 TYPES OF SMS USED IN EVS

EVs are becoming rapidly popular because of its numerous benefits over traditional combustion engine vehicles. EVs offer a cleaner and more sustainable mode of transportation, reducing carbon footprints and dependence on conventional fuels. However, the development of EVs has brought about a new challenge: the need for SMs.

SMs are serving vital role in the development of EVs. Here, we will focus on some of the types of SMs that are commonly applied in EVs [10–12].

13.3.1 SHAPE-MEMORY ALLOYS (SMAs)

SMAs are those materials which can change their shape when exposed to heat or stress. These alloys can be used in various components of an EV, like sensors and actuators. For example, SMAs can be used to develop sensors that can detect changes in temperature or pressure, which can be used to monitor the performance of the vehicle.

They can be used in EVs for a variety of purposes, such as in the development of self-repairing systems, in sensors and actuators, and in the control of vehicle vibration and noise.

13.3.2 PIEZOELECTRIC MATERIALS

Piezoelectric materials are those materials which produce an electric charge when it subjected to mechanical stress. Such materials can be used in various components of an EV-like actuators. These materials may be used to develop sensors that can detect changes in pressure or acceleration, which can be used to monitor the performance of the vehicle.

13.3.3 SHAPE MEMORY POLYMERS (SMPs)

SMPs are those materials which may change its shape when explore to heat or stress. SMPs can be used in various components of an EV, such as sensors and actuators. For example, SMPs can be used to develop sensors that can detect changes in temperature or pressure, which can be used to monitor the performance of the vehicle.

They can be used in EVs for various purposes, such as in the development of self-repairing systems and in the creation of sensors and actuators.

EVs offer a cleaner and more sustainable mode of transportation. However, the development of EVs has brought about a new challenge: the need for SMs.

13.3.4 ELECTROACTIVE POLYMERS (EAPs)

EAPs are those materials which may change its size and shape when subjected to an electric field. EAPs can be used in various components of an EV. For example, EAPs can be used to develop sensors that can detect changes in pressure or temperature, which can be used to monitor the performance of the vehicle [13].

13.3.5 THERMOELECTRIC MATERIALS

Thermoelectric materials are materials that can generate electricity from a temperature difference. These materials can be used in various components of an EV, such as the battery or the exhaust system. Thermoelectric materials may be used to convert the waste heat energy from the exhaust system into electricity, which can be used to power various components of the vehicle [14].

13.3.6 MAGNETORHEOLOGICAL FLUIDS (MRFs)

MRFs are those materials which change its viscosity as a reflex to a magnetic field. Such fluids can be used in various components of an EV, such as the suspension system or the braking system. For example, MR fluids can be used to develop shock absorbers that can adjust their damping qualities as reflex to make changes in road conditions.

13.3.7 ELECTROCHROMIC MATERIALS

These are SMs which can change their pigment as a reflex of an electric charge. These materials may be applicable in EV windows to adjust the light which enters into the vehicle and to reduce the need for air conditioning, thus improving energy efficiency.

13.3.8 THERMOELECTRIC MATERIALS

Thermoelectric appliances are SMs which may produce an electric current when kept to a temperature gradient. It may be used in EVs to reuse waste thermal energy from the engine or exhaust system into electrical energy, which can be used to power the vehicle or recharge the battery [15].

13.3.9 MAGNETIC SHAPE MEMORY ALLOYS

These are the alloy based SMs which may adjust its shape as reflex to a magnetic field. It may be used in EVs for various purposes, such as in the development of adaptive suspension systems, which can adjust the vehicle's ride height and stiffness based on road conditions.

13.3.10 CONDUCTIVE POLYMERS

Conductive polymers are the substance which may conduct electricity and alter its electrical properties as reflex to external stimuli. They can be used in EVs for various purposes, such as in the development of flexible and lightweight batteries and in the creation of sensors and actuators.

13.3.11 SELF-HEALING MATERIALS

These are substances that may heal own selves when caused damage. These materials are applied in various applications in EVs, such as in the car's body panels. These may help to reduce the need for repairs and replacements, minimizing the impact of environment of manufacturing and disposing of materials as well [16].

13.3.12 SUPERCONDUCTORS

Superconductors are materials that can conduct electricity with zero resistance. Superconductors can be use in so many applications in EVs, for example, in the motor and power electronics. Superconducting materials can help improve the efficiency and performance of the EV's components, reducing energy consumption, and improving range.

EVs are becoming rapidly handy due to its various benefits over traditional combustion engine vehicles. EVs offer a cleaner and more sustainable mode of transportation, reducing carbon footprints, and dependency on conventional fuels. However, the development of EVs has brought about a new challenge: the need for SMs [16].

For example, researchers have developed SMs that can help prevent the degradation of the battery. These materials can sense the need of recharging the battery and adjust the charging rate accordingly, reducing the likelihood of overcharging or undercharging. This practice can extend the life span of battery. Specification and application of some SMs are listed in Table 13.1.

TABLE 13.1 SMs with Their Specification ⏎

Smart Material (SM)	Specification	Application in EVs
SMAs	Returns to original shape whensubjected to heat	Regulates the opening and closing of vents, flaps, and valves. Used in shock absorbers and suspension systems to enhance stability and ride comfort
MRF	Changes viscosity and flow behavior when exposed to amagnetic field	Used in EV dampers andshock absorbers to adjust damping force and improve handling and ridecomfort
EAP	Changes shape or size whensubjected to an electric zone	Used in EV sensors, actuators, and motors to improveperformance and efficiency
Piezoelectricmaterials	Generates electricity when expose into mechanical stressor pressure	Used in EV tire pressure sensors, regenerative braking systems,and energy harvesting systems
Thermoelectricmaterials	Converts heat into electricity	Used in EV waste heat recovery systems to improve energyefficiency and reduce emissions
Photochromicmaterials	Changes color or opacitywhen exposed to light	Used in EV windows andsunroofs to regulate the amount of light entering the cabin and improve driver visibility and comfort
Nanomaterials	Unique properties due to smallsize and high surface area	Used in EV batteries, supercapacitors, and fuel cells to improve performance, durability, and efficiency

In addition to the battery, SMs can also be used in other components of the vehicle, such as the tires. Tires are responsible for providing traction and stability to the vehicle, and the properties of the tire may have a significant effect on the overall efficiency of the vehicle. SMs can be used to develop the tires that can adapt to different road conditions, providing better traction and reducing wear and tear.

SMs can also be used in the body of the vehicle. For example, researchers have developed SMs which may adjust their color with respect to thermal conditions. This may be used to apply coatings that can help regulate the temperature inside the vehicle, minimize the requirement of air conditioning that can improve mileage of vehicle.

One of the key components of an EV is the battery. Batteries are responsible for storing and providing power to the electric motor, and the performance of the battery is critical to the overall performance of the vehicle. SMs may be taken to enhance the efficiency as well as durability of the battery.

For example, researchers have developed SMs that may help prevent degradation of the battery. These materials can adjust the charging rate accordingly, reducing the likelihood of overcharging or undercharging. Some of the SMs are trying to show important parts of EV in Figure 13.1.

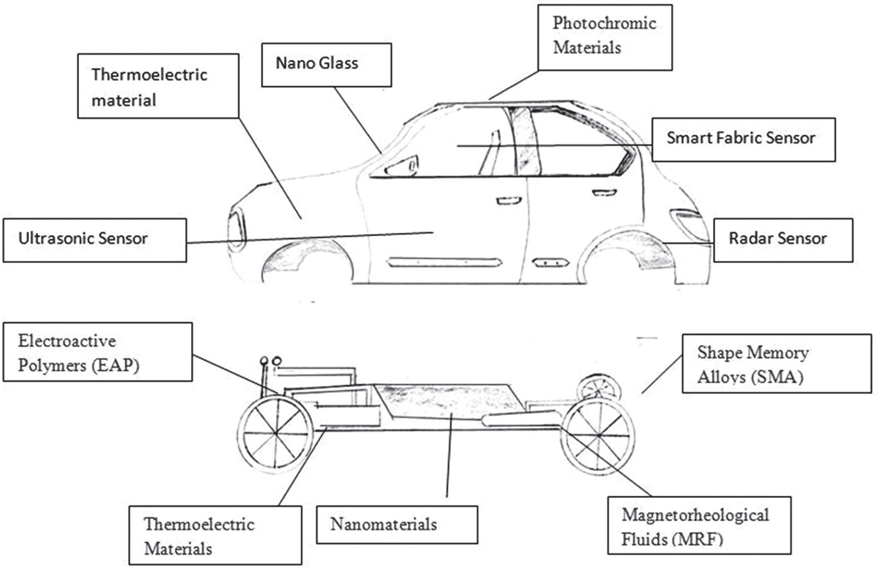
Photochromic Materials
Nano Glass
Thermoelectric material
Smart Fabric Sensor
Ultrasonic Sensor
Radar Sensor
Electroactive Polymers (EAP)
Shape Memory Alloys (SMA)
Thermoelectric Materials
Nanomaterials
Magnetorheological Fluids (MRF)

FIGURE 13.1 Some basic SMs used in EVs. ⏎

EVs are becoming customer friendly because of their numerous benefits over traditional combustion EVs. EVs offer a cleaner and more sustainable mode of transportation. However, the development of EVs has brought about a new challenge: the need for SMs. These materials have unique properties that can be utilized to enhance the performance of various devices, including EVs.

13.4 IMPROVING VEHICLE EFFICIENCY WITH SMS

As the world shifts toward a more sustainable future, the automotive industry is increasingly focused on improving vehicle efficiency. SMs have emerged as a promising solution to this challenge, with their unique qualities which may be utilized to enhance the performance of different vehicle parts. Following are some of the ways in which SMs may be used to enhance vehicle efficiency.

13.4.1 LIGHTWEIGHT MATERIALS

The weight of a vehicle is a crucial factor that affects its fuel efficiency. SMs like carbon fiber, Al, and Mg are lightweight that can be used in various applications, such as body panels, engine components, and suspension systems. These SMs may reduce the weight of the vehicle, increasing fuel efficiency, and help to mitigate emissions.

13.4.2 ENERGY-HARVESTING MATERIALS

These materials can change wasted form of energy into usable energy. For example, piezoelectric materials can convert mechanical energy, such as vibrations from the vehicle's suspension system, into electricity. This electrical energy can be utilized to power the vehicle's accessories or recharge the battery, reducing the load on the engine, and improving fuel efficiency.

13.4.3 THERMOELECTRIC MATERIALS

These SMs may produce electric power when a temperature gradient is applied across them. These materials can be used to capture waste heat and transform it into electrical energy, that may be utilized to power the vehicle's accessories or recharge the battery. By utilizing waste heat, thermoelectric materials can improve fuel efficiency and reduce emissions.

13.4.4 SELF-HEALING MATERIALS

These SMs may auto repair if damaged. These materials may be utilized in various applications, such as body panels, to reduce the need for repairs and replacements. By mitigating the demand for maintenance and replacements, self-healing SMs can help reduce the environmental impact of manufacturing and disposing of materials.

13.4.5 ACTIVE AERODYNAMICS

These SMs are SMAs and electrochromic goods can be used to develop active aerodynamic systems. These systems can adjust the shape and surface properties of the vehicle in real-time, reducing drag and improving fuel efficiency. For example, active grille shutters can be used to close the grille when the engine does not need cooling, reducing drag, and improving fuel efficiency.

13.4.6 SMART TIRES

Tires are a crucial component of a vehicle that affects its fuel efficiency. Smart tires can be developed using materials such as piezoelectric materials and self-healing materials. Piezoelectric materials can be used to measure the pressure in the tires, providing real-time feedback to the driver. Self-healing materials can be used to repair punctures and reduce the need for replacements.

13.5 ENHANCING VEHICLE SAFETY WITH SMS

In recent years, advancements in SMs have provided a new avenue for improving the safety of vehicles. These SMs have the property to find and reply to changes in their environment, providing an added layer of protection for drivers and passengers. From adaptive suspension systems to self-healing coatings, SMs are changing the game when it comes to vehicle safety.

The most promising use of SMs in the automotive industry is in the development of crash avoidance systems. These systems use sensors and algorithms to detect potential collisions and alert the driver or take action to prevent the crash. SMs can enhance these systems by providing more accurate and responsive sensors, as well as materials that can actively absorb impact energy to reduce the severity of a crash.

One of the good examples of an SMs that has been used in crash avoidance systems is SMAs. They have the tendency to recognize their native shape and reform to it if subjected to heat or an electrical current. In a crash avoidance system, SMAs can be used to actuate brakes or steering systems to prevent a collision. This technology has already been incorporated into some high-end vehicles, and is expected to become more widespread as the cost of SMAs decreases.

Another use of SMs in vehicle safety is development of adjustable suspension setup. These systems use sensing device and actuators to manage the stiffness of a vehicle's shock up, on the basis of conditions of road and driving mode. SMs may be used in these systems to produce variable stiffness materials that can adjust their properties on the fly. For example, a material that is stiff at low speeds and soft at high speeds could provide better handling and stability in a wide range of driving conditions.

Self-healing coatings are another area where SMs can enhance vehicle safety. These coatings use materials that can repair damage to the surface of a vehicle, such as scratches and chips, without the need for manual intervention. This not only improves the appearance of the vehicle, but can also prevent rusting and other forms of corrosion that may deform the mechanical integrity of vehicle over time.

Overall, SMs have the tendency to revolutionize vehicle safety by providing new ways to detect and reflex to alter in the vicinal atmosphere. From crash avoidance systems to adaptive suspension systems and self-healing coatings, these materials are already being incorporated into vehicles at the high end of the market, and are expected to become more widespread as the cost of these materials decreases. As these technologies become more accessible, we can look forward to a future where vehicles are safer, more efficient, and more environmental friendly than ever before.

Vehicle safety has come a long way since the first automobiles were invented. With advances in technology, cars have become safer with features like seatbelts, airbags, and backup cameras. However, there is always room for improvement, and one area that has the potential to enhance vehicle safety is SMs [17].

One potential application for SMs is in vehicle safety. By mixing SMs into various components of a car, manufacturers could improve safety features and reduce the risk of accidents on the road.

One of the examples of an SMs that could be used in vehicles is SMAs. These are metals which may “remember” its native shape and size and reform again after being damaged. This property could be used in various safety features, such as a bumper that can absorb impact and reform again to its original position after a collision.

Also SMs that could be used in vehicle safety is piezoelectric materials. Piezoelectric materials generate electricity when they are exploring to structural stress.

By incorporating these materials into the tires of a car, for example, they could generate electricity as the car drives over the road, which could be used to power various safety features, such as headlights or warning signals.

SMs could also be used to create sensors that can detect changes in temperature, pressure, or other factors that could indicate a potential safety issue. For example, a sensor could detect a change in tire pressure and alert the driver to the need for maintenance or replacement.

In addition to improving safety features, SMs could also be used to make vehicles more comfortable and convenient. SMs could be utilized to produce seats that adjust to the individual driver’s body shape and position, reducing the risk of fatigue and discomfort during long drives.

There are also potential environmental benefits to using SMs in vehicles. By reducing the weight of various components, such as the body or engine, vehicles could become more fuel-efficient, reducing emissions and contributing to a cleaner environment.

SMs, also called intelligent materials, have revolutionized the way we design and manufacture products. They may change their character as a reflex to changes in their environment. SMs have various uses, including enhancing vehicle safety.

Safety of a vehicle and its passengers has always been a big concern for all automobile industry. By the increasing automobiles on the road, accidents have become more frequent. To address this issue, automakers have been constantly introducing new safety features in their vehicles. SMs have played a crucial role in enhancing these safety features.

The most common use of SMs in vehicles is in airbags. Airbags are designed to deploy in case of a collision, protecting the occupants of the vehicle from injury. SMs are used in airbags to improve their effectiveness. They are used to create airbags that can adjust their deployment speed based on the severity of the collision. This ensures that the airbags do not deploy too early or too late, minimizing the risk of injury to the occupants.

Another use of SMs in vehicles is in the construction of the body of the vehicle. SMs are used to create materials that can absorb the impact of a collision, reducing the damage to the vehicle and the occupants. These materials are also used to create lightweight, yet strong, materials that can improve fuel efficiency while maintaining safety. Some important SMs are listed in Table 13.2 with their chemical name and working temperature.

TABLE 13.2 SMs with Their Chemical Name and Working Temperature ⏎

Smart Material (SM)	Example	Working Temperature Range
SMAs	Nitinol	–200 to 100°C
MRF	Ferrofluids	–40 to 90°C
EAP	Polyvinylidene fluoride	–40 to 60°C
Piezoelectric materials	Lead zirconate titanate	–55 to 150°C
Thermoelectricmaterials	Bismuth telluride (Bi_2Te_3)	–40 to 700°C
Photochromic materials	Glass containing silver halide crystals	–40 to 80°C
Nanomaterials	Carbon nanotubes	Varies

Note: Working temperature ranges may change depending on the particular substance, application, and manufacturer, so this table provides general guidelines. It's always important to check the specifications and requirements for a specific SM and application to ensure optimal performance and safety.

SMs are also used in the design of sensors and control systems in vehicles. They are used to create sensors that can detect changes in the environment, such as changes in temperature or pressure. These sensors are then used to control various systems in the vehicle, such as the brakes or the steering, ensuring that the vehicle responds appropriately to changes in the environment.

13.6 SMS AND VEHICLE SUSTAINABILITY

The automotive industry is one of the largest contributors to greenhouse gas emissions, with vehicles responsible for a significant portion of carbon dioxide emissions worldwide. As concerns about climate change and sustainability continue to grow, there is an urgent need to find ways to mitigate environmental issues of vehicles. One potential solution is the use of SMs in vehicles, which can improve their sustainability and reduce their carbon footprint.

13.6.1 ENERGY EFFICIENCY

The key benefits of SMs in vehicles are their ability to improve energy efficiency. SMAs may be utilized to produce lightweight components which may convert structure as a reflex of temperature gradients, reducing the need for heavy hydraulic systems. This can result in significant fuel savings and reduced emissions.

Similarly, phase change materials (PCMs) can be taken to capture and release thermal energy, helping to regulate the temperature within the vehicle. This reduces the need for heating and cooling systems, resulting in improved energy efficiency and reduced emissions.

13.6.2 LIGHTWEIGHTING

SMs may also be utilized to mitigate the weight of vehicles, which is critical in improving fuel efficiency and reducing emissions. For example, CFRP is an SM which is lightweight and strong, proving it the best substance for use in the body of vehicles. By using CFRP, vehicle manufacturers can reduce the weight of vehicles, improving their fuel efficiency and reducing their carbon footprint.

13.6.3 DURABILITY

Another benefit of SMs in vehicles is their durability. Self-healing materials, for example, can detect and repair damage automatically, reducing the need for maintenance and repair. It mitigates the environmental issues of vehicle maintenance and also improves the lifespan of the vehicle.

13.6.4 RECYCLING

SMs may also improve the recyclability of vehicles. For example, thermoplastic composites can be melted down and reused in the manufacturing of new components. This reduces waste and minimizes the need for raw materials, improving the sustainability of the manufacturing process.

13.7 CHALLENGES AND LIMITATIONS OF SMS IN EVS

SMs have been identified as a promising technology to enhance the performance of EVs. Their ability to respond to outer action, like thermal and pressure impact and magnetic fields make them best material for application in different applications, including energy storage, thermal management, and structural materials. However, the use of SMs in EVs is not without its challenges and limitations.

13.7.1 COST

One of the noticeable challenges of using SMs in EVs is the cost. SMs, like SMAs and CFRPs, are expensive to manufacture and process. The big cost of SMs makes it difficult to produce EVs that are affordable for the general population. As a result, many EV manufacturers may choose to use traditional materials, such as steel or aluminum, which are less expensive but may not provide the same benefits as SMs.

13.7.2 INTEGRATION

Another challenge of using SMs in EVs is the integration of these materials into existing manufacturing processes. The production of EVs requires a complex supply chain and an extensive infrastructure to support it. The integration of SMs into this system may require significant changes to manufacturing processes, equipment, and facilities. This can be a time-consuming and costly process, which may deter manufacturers from adopting SMs in their vehicles.

13.7.3 RELIABILITY

SMs also have limitations when it comes to reliability. The performance of SMs can be affected by environmental impact, like humidity, and their response may be unpredictable. For example, SMAs can experience fatigue after repeated use, which can affect their tendency to reform in their natural structure. This can be problematic in applications where reliability is critical, such as in structural components or safety systems.

13.7.4 REGULATORY APPROVAL

SMs may also face challenges in obtaining regulatory approval. The utilization of recent materials in EVs requires certification and approval by regulatory bodies, like the National Highway Traffic Safety Administration in the United States. These agencies may require additional testing and data to ensure the safety and performance of new materials, which can be a time-consuming and costly process.

13.8 FUTURE DIRECTIONS FOR SMS IN EV ADOPTATION

The acceptance of EVs has been on demand in last few years, and with it comes a rise for innovative solutions to improve their performance, efficiency, and sustainability. Here, we will explore the future directions for SMs in EV adoption.

13.8.1 ENERGY STORAGE

The tightest provocation that is opposing by the EV industry is limited range of EVs compared to their gasoline counterparts. SMs offer a solution to this problem by improving the energy storage capacity of EVs. One such material is graphene, which has excellent conductivity and can be used to create supercapacitors with high energy density. These supercapacitors can charge and discharge quickly, reducing the charging time for EVs and extending their range.

Another SM that can enhance energy storage in EVs is lithium–sulfur batteries. Lithium–sulfur batteries offer a higher energy density than traditional lithium-ion batteries and are also cheaper to produce. These batteries also have the potential to be made more sustainable by replacing the toxic and scarce cobalt used in lithium-ion batteries with sulfur.

13.8.2 THERMAL MANAGEMENT

Heat management is another area where SMs can play a significant role in EVs. EVs generate a lot of heat, which can damage components and reduce their lifespan. SMs like SMAs and PCMs can be used to manage the heat generated by EVs. SMAs have the ability to change shape when exposed to heat, allowing them to act as heat sinks and dissipate the excess heat. PCMs, on the other hand, can absorb heat when the temperature rises and release it when the temperature falls, thereby maintaining a stable temperature within the EV.

13.8.3 STRUCTURAL INTEGRITY

SMs can also improve the structural integrity of EVs. For instance, CFRP is a SM that is lightweight and strong, proving it best in utilization in the body of EVs. CFRP may enhance the safety of EVs by reducing their weight and improving their crash resistance.

13.8.4 SELF-HEALING MATERIALS

These are another segment of SMs which can enhance the durability and lifespan of EVs. These may detect and repair deforms parts automatically, reducing the necessities of further maintenance and repair. These materials can be used to create components such as tires, which can repair themselves when punctured, reducing the frequency of tire replacements.

13.9 CONCLUSION

In conclusion, SMs can prove as powerful tool to create a new era of the EV industry by transforming them easy affordable and more sustainable. As the demand for EVs grows, there will be a need for new and innovative materials to address the challenges faced by the industry. The development and adoption of SMs can help accelerate the transition to a cleaner and greener future.

The research on SMs is crucial for the advancement of EVs. SMs can provide a combination of lightweight, high-strength, and self-healing properties, improving the efficiency and safety of EVs. One can also be use these materials to transform waste thermal energy into electricity, reducing energy losses and improving the range of EVs. As the demand for sustainable transportation grows, the development of SMs will have a key role in manufacturing of EVs more practical and affordable for customer.

The development of EVs has brought about a new challenge: the need for SMs. SMs may be utilized to enhance the effect, efficiency, and durability of various components of the vehicle.

By utilizing these materials, we can improve the efficiency, durability, and performance of EVs, and reduce their environmental impact. The above-mentioned types of SMs are just a few examples of the diverse range of SMs that can be used in EVs, and we can expect to see even more innovative uses of SMs in the future.

SMs have the power to transform the performance and sustainability of EVs. They can improve energy storage, thermal management, light weighting, and durability, all of which are critical in enhancing the efficiency and range of EVs. The integration of SMs into the design and manufacturing of EVs represents an exciting opportunity to advance the automotive industry and come up with a more viable future. As soon as technology pursues to evolve, the full potential of SMs in EVs is yet to be realized.

SMs have the potential to significantly improve vehicle efficiency. Lightweight materials, energy-harvesting materials, thermoelectric materials, self-healing materials, active aerodynamics, and smart tires are just some of the ways by which SMs can be utilized to improve vehicle efficiency. As the demand for more sustainable vehicles continues to grow, the development and application of SMs shall prove an increasingly key bit character in the expansion of more efficient and sustainable vehicles.

While the technology is still in its early stages, continued research and development in this area could lead to a new era of automotive innovation and safety. They utilized in different applications, together with airbags, body design, sensors and control systems, and self-healing materials. With the continued development of SMs, we can expect to see even more advanced safety features in vehicles in the future.

They can improve energy efficiency, reduce weight, enhance durability, and improve recyclability. By incorporating SMs into the design and manufacturing of vehicles, we may mitigate the sustainable effect of transportation and move toward a more viable life of human being. Since automotive industry moving on to evolve, the use of SMs will become increasingly important in achieving this goal.

The use of SMs in EVs has significant potential to improve their performance and sustainability. However, the challenges and limitations of SMs, including their cost, integration, reliability, and regulatory approval, must be addressed to ensure their widespread adoption in the automotive industry. Manufacturers and researchers must move on to develop inventive course of action to overcome these challenges and unlock the full potential of SMs in EVs. Only then we can achieve the goal of sustainable, efficient, and reliable EVs.

SMs also proved a powerful tool evolution of the EV industry by improving energy storage, thermal management, structural integrity, and durability. Graphene, lithium–sulfur batteries, SMAs, PCMs, CFRP, and SHMs are just a few examples of SMs which can be used in EVs. As the demand for EVs continues to grow, the development of SMs will become increasingly important in ensuring the performance, efficiency, and sustainability of these vehicles. The future of EVs is bright, and SMs will play a crucial role in shaping it.

KEYWORDS

- **smart materials**
- **electric vehicles**
- **batteries**
- **energy storage**
- **vehicle sustainability**

REFERENCES

1. Dang, H., Tian, X., Jiang, C., Chen, S. Recent progress in the development of smart materials for energy storage applications. *J. Mater. Chem. A*, **2021**, *9*(8), 4479–4500.
2. Alam, M.N., Rahman, M.A., Akhtaruzzaman, M., Rashid, M.T. Electric vehicles: a review on battery management systems. *J. Energy Storage*, **2019**, *22*, 100781.
3. Andreescu, S., Sadarangani, C., Schiz, J.F. Smart materials for energy harvesting and storage: a review. *Mater. Sci. Eng. R: Rep.*, **2020**, *140*, 100538.
4. Chen, L., Sun, J., Zhang, J. Materials science for rechargeable batteries. *Front. Energy Res.*, **2019**, *7*, 141.
5. Debnath, B., Bhattacharyya, S. A comprehensive review of energy management strategies for electric vehicles. *Renew. Sustain. Energy Rev.*, **2021**, *135*, 110248.
6. Dong, Y., Li, Z., Chen, L. Progress in the development of smart materials for energy conversion applications. *J. Mater. Chem. A*, **2019**, *7*(31), 18267–18293.
7. Guo, X., Zhang, Q., Wang, Q. Applications of smart materials in renewable energy technologies: a review. *J. Renew. Sustain. Energy*, **2019**, *11*(3), 033102.
8. Hu, Y., Liao, L., Wu, Y. Smart materials for high-performance energy conversion and storage devices. *Prog. Mater. Sci.*, **2019**, *99*, 481–521.
9. Hu, Z., Chen, W., Chen, L. Smart materials for solid-state lithium-ion batteries: recent progress and perspectives. *J. Energy Chem.*, **2020**, *45*, 135–146.
10. Huang, H., Zhang, B., Wang, Y. Progress and prospects of smart materials for solid-state electrolytes in rechargeable batteries. *J. Energy Chem.*, **2020**, *45*, 1–16.

11. Huo, J., Su, G. Smart materials for energy harvesting and sensing applications: a review. *Smart Mater. Struc.*, **2020**, *29*(8), 083001.
12. Jena, A., Reddy, B.S. Review on smart materials for energy harvesting and storage applications. *Mater. Today Proc.*, **2019**, *14*, 328–335.
13. Khajuria, D.K., Kumar, V., Kumar, A. A review on smart materials for energy storage and conversion applications. *J. Energy Storage*, **2021**, *36*, 102287.
14. Liu, Q., Zhang, G., Wei, X. Smart materials for energy-saving buildings and sustainable energy systems. *Renew. Sustain. Energy Rev.*, **2019**, *111*, 411–424.
15. Loh, G.C., Wang, C.H. A review of battery technologies for electric vehicles. *Energy*, **2021**, *223*, 120048.
16. Lu, X., Wang, L., Xia, Y. Smart materials for rechargeable batteries. *J. Energy Chem.*, **2020**, *45*, 90–101.
17. Wen-Yeau, C. *The state of charge estimating methods for battery: a review*. Hindawi, **2013**. http://dx.doi.org/10.1155/2013/953792.

CHAPTER 14

RHEOLOGY OF SMART MATERIALS IN SCIENCE AND ENGINEERING FIELDS: AN INDUSTRIAL PERSPECTIVE

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ABSTRACT

Smart materials are designer, task-specific, or external stimuli-responsive materials. These intelligent materials' behaviors can be remarkably tuned by changing their pH, moisture, temperature, pressure, electric and magnetic fields, light, or compositions of chemical compounds. To design smart materials spectacularly, the required components are highly integrated. These sharp-witted materials fulfil the needs of the environment and most of the industrial requirements. The development of these high-end materials does not require more space, a typical operating environment, time, or costs. Right from its discovery, its divergence varies from designing smart infrastructures, sensors, gadgets, and even to smart vehicles. The most important property of these smart materials, which are mostly followed in the new technological era, is due to their stimuli response to the external force. Smart materials are the combinations of more than one material, which are also known as smart memory alloys (SMAs), which are mainly responsible for the smart memory effect. This chapter aims to portray the most important factors, which appeal to these SMAs as smart materials in science, technical, and engineering applications. Industrial perspectives include aerospace,

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automotive, mini actuators, robotics, microelectrochemical systems, and structure and composites in a detailed manner.

14.1 INTRODUCTION

Right from ancient days, the evolution of human beings is directly connected to their civilization and is precisely intertwined with the method of living to materials they used for their various walks of life. Since the nature of the materials adopted for their livelihood describes their standard of life. Every interpretation of each stage of civilization is one way or another way related to material development. In fact, materials used in different era describe the level of civilization of the particular century. The present twenty-first century may be considered the development of the multifunctional materials age.

The contemporary twenty-first century is being raised to a higher rank or position in science and technology. In the present scenario, there are number of new fields and disciplines emerging in a new way that leads to the futuristic development of materials with the utilization of new age technology with novel applications. These materials are generally considered as smart materials. The emergence of these advanced materials is nothing but existing habitual materials. Their existing properties have been amplified with the help of high-end technology, by increasing their performance in a remarkable way that can lead to a significant role in the enhancement of the society. Typical advanced materials include all types of materials including ceramics, metals, polymers, semiconductors, and biomaterials and are normally expensive and described as “Materials of the Future.”

Smart and nano-engineered substances are generally recognized as advanced materials. The extension of nanoscience and nanotechnology during recent times reinforces the establishment of smart materials which are otherwise considered “designer materials” or “intelligent materials” and will lead most of a significant influence on most of the existing technologies.

To design this highly integrated smart material in a technically advanced manner, one requires sound interdisciplinary knowledge. Smart materials are designated as intelligent or responsive materials that can be designed according to one’s desire. Properties of these materials can be manipulated and can be made to respond in a controllable and reversible way through external stimuli such as certain mechanical stress or a certain temperature [1].

According to NASA, smart materials possess specific configuration and have the ability to respond to the external stimuli, without losing its original properties [2–7].

These smart materials have some specific inbuilt properties that can react according to the external stimuli response, to complete the desired task. Scientists named these materials as advanced, intelligent, or even adaptive materials, whose features are generally venerable to normally existing materials. Some of their unique characteristics are represented as follows [8–10].

1. *Transiency:* React according to the motive and able to stay in different states.
2. *Proximity:* React immediately with external stimuli without wasting much time.
3. *Self-inclination:* React according to the materials' inner response.
4. *Discernment:* React in a distinguished and predictable manner.
5. *Ingenuousness:* Reaction and action occur simultaneously in the same place.

The distinctive nature of these intelligent materials are obtained as a result of their competence and can change its intriguing property according to external stimuli by integrating the functionality in their structures, thereby enhancing their internal structure and form. Obviously, these stimulant-activated materials are used to respond to change its external factors like opacity, flexibility, humidity, porosity, and electrical properties like electronics and other fields.

The amalgamation of smart structures and the inbuilt nature of these intelligent materials are mainly for their stimuli-sensitive property of these intelligent materials. Hence, these, intelligent materials possess the properties to respond and receive any kind of signal from the environment as well as from their inner properties. Accordingly, they adopt their changes by consolidating the required function in their structure. In recent times, the attraction of smart materials is flourishing due to their demand in various fields such as aerospace, actuators, sensors, and so on.

In 1968, Clauser [11, 12] discovered the basic idea of synthesizing smart materials and elevated the concept behind it. However, only after 1990, the field flourished as an active field. Understanding the basic concepts and behavior of smart materials lends their widespread utility as commercial products in the form of piezoelectric, polycrystalline piezoceramic including electrostrictive, magnetostrictive, shape memory alloys (SMAs), and electrorheological (ER)/magnetorheological (MR) fluids [13].

The schematic representation of the action of these intelligent materials with respect to the influence out word surroundings is depicted in Figure 14.1. Generally, smart materials behave as replicas of most of the naturally existing systems. According to a previous study [14], smart materials possess distinctive properties as it can adopt both mechanical and nonmechanical characteristics and hence confers its applications in a widespread way.

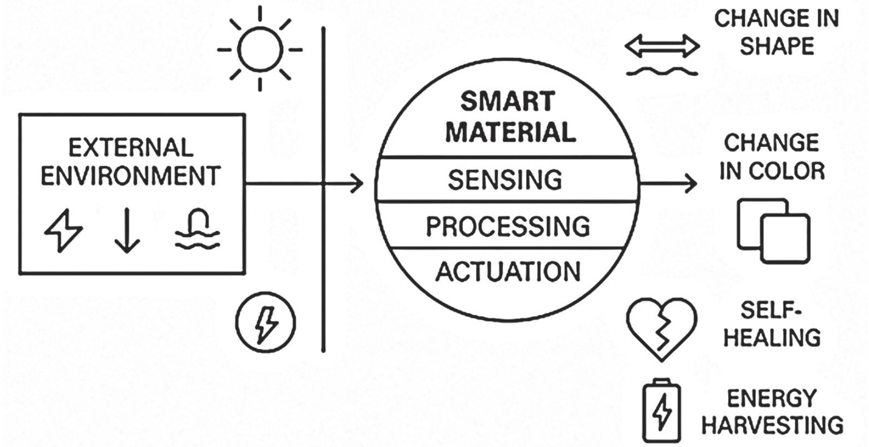

FIGURE 14.1 Action of smart materials with respect to influence of external environment. ⏎

14.2 CLASSIFICATIONS OF SMART MATERIALS

In a broader way, smart materials are classified as active or passive. Smart materials are called active in the sense that their ability to modify their geometric properties under the influence of external stimuli, enhancing their inherent properties.

Based on their response to the respective domain, smart or intelligent materials are further categorized as follows [15]:

1. *SMAs:* Acts with respect to pressure and heat.
2. *ESMs:* Acts with respect to the electric field.
3. *MSMs:* Acts with respect to the magnetic field.
4. *CMs:* Acts with respect to electrorheological fluid.
5. *ERF:* Acts with respect to the electric field and.
6. *MRFs:* Act with respect to the magnetic field.

14.2.1 SMA

SMAs or “smart alloys” are smart materials, which possesses two basic phases and can change these phases by the impact of circumstantial forces such as temperature or stress. These SMAs have specific compositions of alloys and can attain their native shape, which is considered as shape memory transformation [16] or SMAs. These SMAs are generally lightweight solid particulars and are persistent to act as of efficient actuators, and such kinds of actuators are hydraulic, pneumatic, or motor based systems [17]

Ölander [18] discovered about the shape recovery of Ag–Cd-based SMAs [19, 20]. Since then, studies have focused on finding the importance and the rheology of these SMAs in a detailed manner. In that way, they found one of the most important, powerful functionality with wide utility in commercial purposes-based effective SMAs such as nitinol alloy system, NiTi [21].

The physical parameters such as differences in temperature influence the enhancement of phase behavior and structure changes of most of the SMAs, which accompany the most enhancing applications compared to most of the conventional materials. Some common SMA systems used in most of the research and industries are shown in Table 14.1 [22–24].

TABLE 14.1 Customary SMA Systems [22–24] ⏎

Alloy	**Compositions**	**Transformation Temperature As, Range (°C)**	**Transformation Hysteresis**
Ag–Cd	44/49 at Cd	−190 to −50	~15
Au–Cd	46.5/50 at Cd	30 to100	~15
Cu–Al–Ni	14/14.5 wt%-Al,3/4.5 wt%Ni	−140 to 100	~35
Polycrystalline	13.5wt%-Ni 4.1wt%	149	~21
Cu–Al–Ni single crystal	Cu 82.4%-Al	157	~12
Cu–Sn	15at%sn	−120 to 30	~10
Cu–Zn	38.5/41.5 wt% Zn	−180 to −10	~10
Cu–Zn–X (X = Si, Sn, Al)	Small wt%	−180 to 200	~10

14.2.2 COMMERCIAL APPLICATIONS OF SMAs

The commercial utility of these SMAs is used in the following fields as follows:

1. *Actuators:* Electrical components like automobiles, robotics, etc.
2. *Smart materials:* Act both as actuators and sensors.
3. *Couplings:* Known for its effective use of SMAs.

The emergence of SMAs increases their demand in science, technology, and engineering fields, including changes in structure and composites [19], industrial usages [25–27], and consumer products such as automotive [28–30], aerospace [31–33], mini actuators [34, 35] and microelectromechanical systems (MEMS) [36].

Some other metals that exist in SMAs are alloying the metals such as zinc, copper, gold, and iron. Although the iron- and copper-based SMAs like Fe–Mn–Si, Cu–Zn–Al, and Cu–Al–Ni are low cost, its brittleness, instability [37–39] and poor thermomechanic performance [40]. The combinations like Cu–Al–Ni and Ni–Ti alloys of SMAs take part in a crucial aspect in most of the industrial executions. SMAs with this type of alloy exhibit crystals with three different basic structures with two types of phases as shown in Figure 14.2 twinned martensite, detwinned martensite, and austenite have transformations [41, 42] with six possible ways. With respect to temperature, these phases undergo a transformation from one phase to another. The corresponding phase transformation with correspond to temperature is depicted in Figure 14.3.

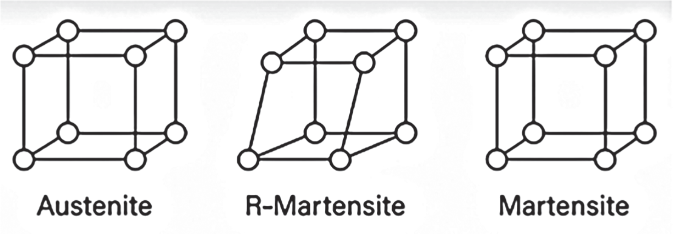

FIGURE 14.2 Three basic crystal structures of SMAs. ⏎

The temperature is responsible for the austenite state (As) phase changes to the corresponding austenite state (Af) corresponds to the final transformation process. SMAs attain their original form, by heating (As) to beyond their temperature, thereby, getting contracted and transforming into the austenite structure. The aforementioned transformations are possible by applying high stuffs and their outcomes are in high actuation energy densities [42] in SMAs. At martensite-start temperature (Ms), the cooling operation will be accomplished when the formation of martensite occurs during the degenerate process. The entire process will be completed when it attains martensite-finish temperature (Mf) and the entire sequence is depicted in Figure 14.4 [44, 45].

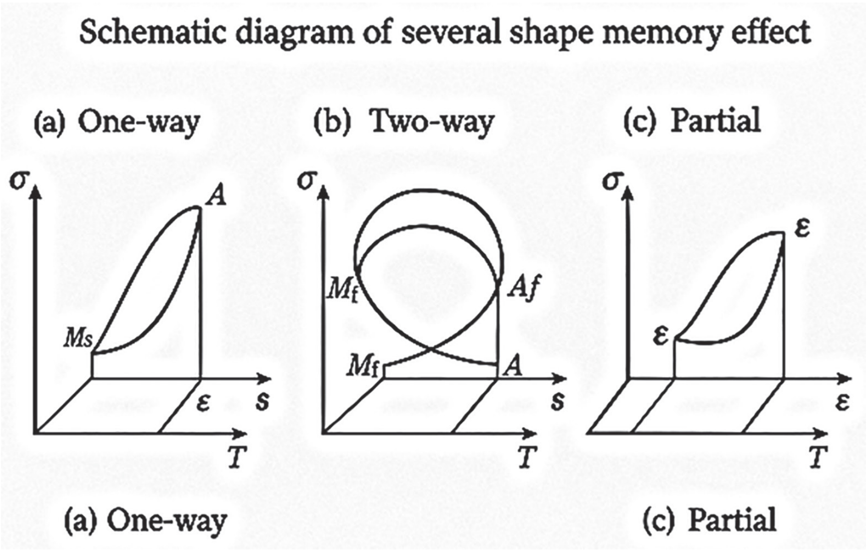

FIGURE 14.3 Illustrative representation of specific SME parameters (stress, strain, and temperature) [43]. ⏎

The maximum temperature at which martensite form can be free of stress is called Md, and above this particular temperature, SMAs will permanently be deformed into any ordinary metal-like material [38]. The transformation of this shape-changing effect is known as shape memory effect or pseudoelastisity.

14.2.3 FERROIC CHARACTERISTICS OF SMAS

The materials with "ferroic" characteristics [47] are considered smart materials like SMAs, piezoelectric, and electroactive polymers that exhibit a strong tendency of merging between the applied electric, magnetic, or thermal field with their mechanical properties (strain, viscosity, etc.). These "ferroic" materials are generally focused on basic physics, structures, material science, and devices and are classified based on their ability to couple with the stimuli and are shown here.

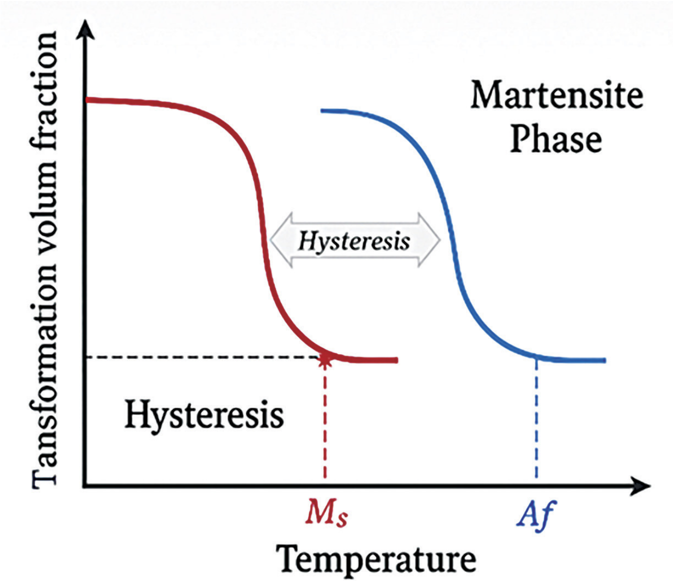

FIGURE 14.4 SMA (HT) phase transformation of Flexinol NiTi [46]. ⏎

1. *Ferroelectric:* Materials which electromechanically coupled with stimuli are known as piezoelectric and those coupled with thermoelectrically with stimuli are known as pyroelectric materials.
2. *Ferromagnetic:* Materials when magnet mechanically coupled with stimuli are known as ferromagnetic materials.
3. *Ferroelastic:* Materials when thermomechanically coupled with stimuli are known as ferroelastic materials.

Hence, those materials which are considered ferroic materials should possess the minimum of any of the above said characteristics of ferromagnetic, ferroelectric, and ferroelastic.

Figure 14.5 depicts the effect of coupling and interaction between ferroic materials and stimuli like electricity, mechanics, magnetism, heat, and optics and leads to many smart functions necessary for most industrial needs.

14.3 ACTUATORS

Actuators are among other smart materials, which had been developed recently. Due to their simple, compact size and unique properties, they exhibit their wide applications in the aerospace industry, automotive systems, biomedical devices, and robotics, to name just a few. Actuators provide vast solutions to most of the pop-up areas such as prosthetics, bio manipulation, implantable drug delivery systems, and scanning probe microscopy.

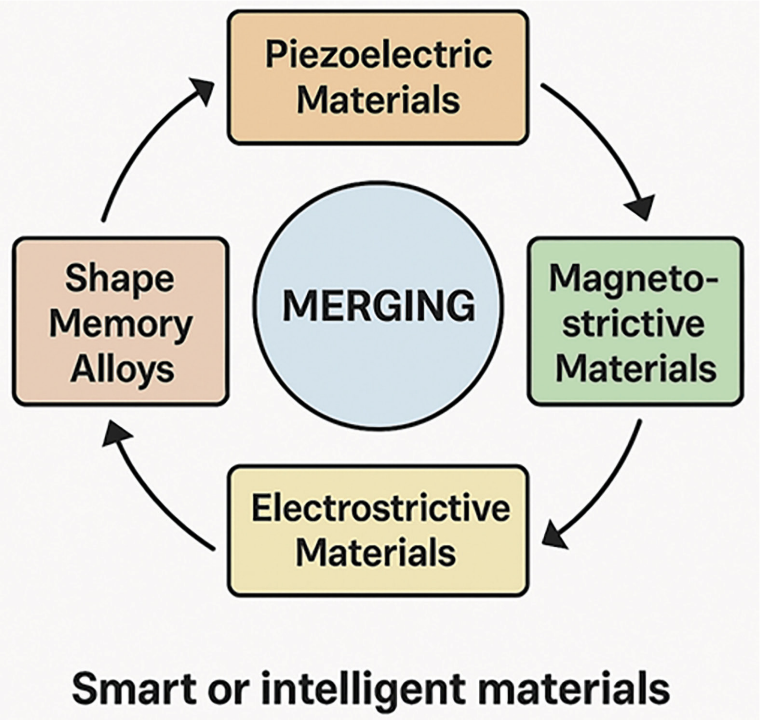
Piezoelectric Materials
Magneto-strictive Materials
Electrostrictive Materials
Shape Memory Alloys
MERGING
Smart or intelligent materials

FIGURE 14.5 Illustrative picture of merging ability of various moduli and their brief categorization of smart or intelligent materials [48]. ⏎

The two basic genres of actuators are conventional and unconventional actuators. The mechatronic systems act as an essential component in conventional actuators (Figure 14.6, left). Examples of conventional actuators are electrical motors, hydraulic pistons, and pneumatic actuators. These systems are not just the intrinsic portion of the system rather they contribute to the structure and sensing, mechanical functions, and actuation (Figure 14.6, right).

Most of the SMAs act as reliable actuators since they possess attractive characteristics elements like sensorial and actuation and are able to function as effective actuators and sensors. The SMAs in two ways have the capability to recognize their high- and low-temperature austenite shapes, whereas the SMAs in one way are able to remember high-temperature shapes only.

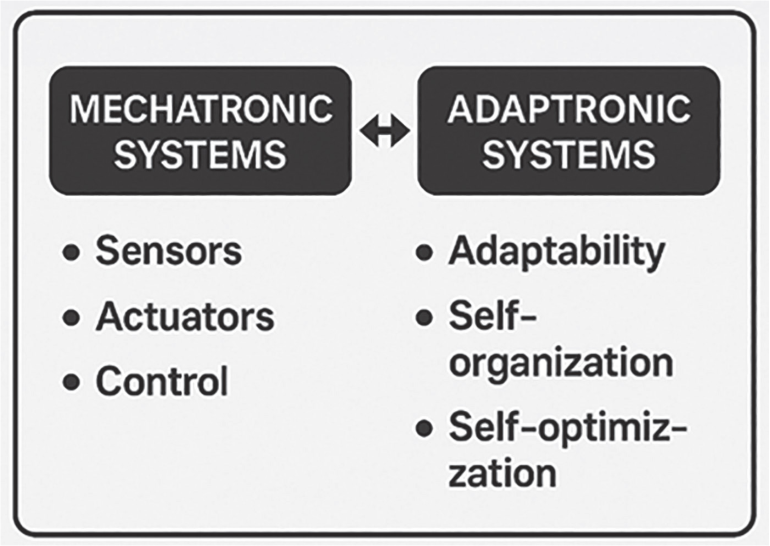

FIGURE 14.6 Characteristics of mechatronic and adaptronic systems [49]. ⏎

SMAs in electrically driven actuators are grouped in two ways—biased and differential (shown in Figure 14.7a) [50]. The figure depicts the principle behind biased actuators 1 and 2. SMA changes force Fa on heating to Fb on cooling in normal actuators. Whereas in biased actuators the driving force is the existence of disparity among these two forces takes place on heating as Fa – Fb and on cooling takes place between Fb – Fm. In the present system, the final force is unsymmetrical and involves two movements in different directions. The biased actuator is also known as a one-way actuator.

Differential actuators, as shown in Figure 14.7b [51], is a symmetrical ones with the final driving force Fa – Fm in the two directions and their end driving force is generally two times that of biased actuators.

These SMAs of actuators can be actuated in many ways such as change in passing electric current through SMA is known as electric actuators, and exposure to atmospheric temperature is known as thermal actuators. The design of these types of actuators with an integrative approach which covers the design of the components is depicted in Figure 14.8 [52].

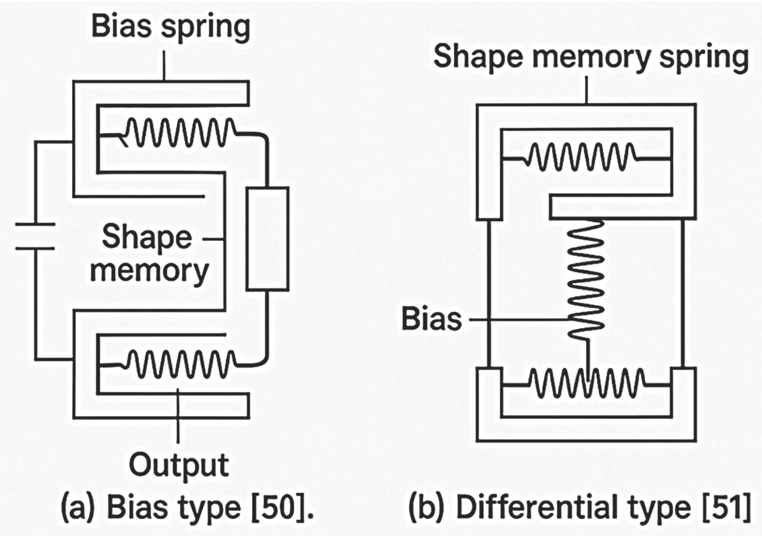
Bias spring
Shape memory
Output
(a) Bias type [50].
Shape memory spring
Bias
(b) Differential type [51]

FIGURE 14.7 The basic techniques of relating shape memory springs to the assembly of electrical actuators: biasing and differential. (a) Bias type [50]. (b) Differential type [51]. ⏎

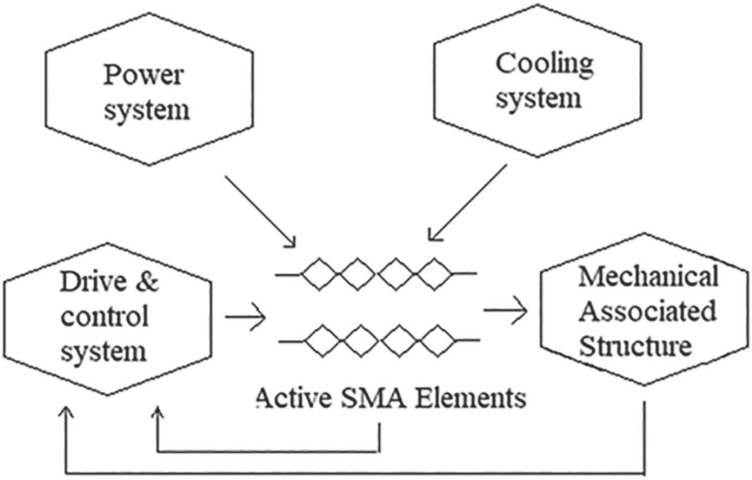
Power system
Cooling system
Drive & control system
Mechanical Associated Structure
Active SMA Elements

FIGURE 14.8 The structure of SMA actuators [52]. ⏎

Generally, actuating systems present in actuators convert energy input into controlled motion. The actuation effects can be achieved in three ways such as field interaction, mechanical interaction, and induced limited strain. Among these actuation effects the one with induced limited strain belongs to smart or intelligent materials.

14.3.1 SMA ACTUATORS AND THEIR ADVANTAGES

The SMA-based actuators are effective compared to most of the existing conventional systems due to the following unique properties they possess:

1. lightweight,
2. small size,
3. low complexity,
4. smooth and silent operation,
5. high power-to-weight ratio, and
6. long life and precise controllability.

These SMA-based actuators' performance is directly related to their environmental temperature and their heat conduction conditions. Apart from that their strain level and cycling sequences also influence the performance sequence of actuators relevant to SMA-based systems.

SMA-based actuators are broadly used in most of the engineering and industrial fields such as the automobile industry [53], aerospace [54], precision engineering, mini- and microrobotics, electrical engineering, aeronautical industry [55], entertainment industry, [56], microelectro-chemical systems, and biomedical engineering. Different types of actuators with working principles and their applications are shown in Table 14.2 and correspondingly different SMA actuator materials and compositions are shown in Table 14.3.

14.3.1.1 UNDERWATER ROBOTS

High-frequency response actuators with exorbitant and low bandwidth of less than 2 Hz [80] function as underwater robotics systems. Since, these actuators when buried in the respective space, exhibit better reaction with respect to the corresponding cooling systems. But the major drawback behind this process is it requires high power to heat actuators.

14.3.2 ACTUATOR–SENSOR SYNTHESIS

There are some systems that are known as self-sensing actuation, in which the same device functions concurrently actuator as well as a sensor. These combined systems are more advantageous for most of the active control systems since both sensing and actuation are perfectly coinage with each other [81].

TABLE 14.2 Different Types of Actuators with Working Principles and Their Applications [57]

S. No.	Type of SMA Actuator	Working Principle	Applications	References
1	Thin film actuator	- Titanium nickel (TiNi) - Diaphragms Type - Thermal actuator	Micropumps in drug delivery system, fuel injection system, etc.	[58, 59]
2	Servo Actuator	- Titanium Nickel (TiNi) with Ti-50.2 at% of Ni. - Microcomputer controlled - Electric resistance feedback control System	Active Endoscope (Medical Robot)	[60]
3	Wire actuator	- Thermal actuator - Control strategy for adjusting wire temperature quickly. - Composites	Active shape control of Inflatable space structures, Automobile safety system, Automobile mirrors, Adaptive control, Mobile microrobots, actuation of aircraft flight surfaces, robot arms and grippers, artificial muscles.	[61–68],
4.	Spring actuator	- SMA helical springs - One-way actuator - Bias mechanism	Active bending system and gripping system, active hand prosthesis, Pipe Robot	[69–71]
		- NiTiCu spring - Actuation gas Temperature viewed	Fire check Valve in industries	[72]
		- NiTi washers used - NiTi TVR spring in pressure sensing device	Gearbox, jet engine oil filters	[73]
5.	Strip actuator	- SMA strip and springs used to achieve output - Planetary system - Automatically driven	Colonoscope robotic arm	[74]

TABLE 14.2 *(Continued)*

S. No.	Type of SMA Actuator	Working Principle	Applications	References
		NiTiCu element - Fluid temperature is actuation parameter	Domestic safety devices	[72]
6.	Ferromagnetic SMA	- Magnetic force actuation - Rapid actuation motion	Actuator, Valves, Biomedical Applications, Hydraulic Pumps	[75–77]
7.	Disc actuators	- Bimetallic actuators	can be used current interrupt mechanism in batteries	[72]
8.	SMA dampers	- Noise and vibrations	Structural supports, Engine mountings	[64, 65]

Piezoelectric materials generally transfer their properties between the electric states (voltage and charge) and the structural states (stress and strain). The incorporation of piezoelectric elements [82] into a bridge circuit will result in a piezoelectric self-sensing actuator. The main objective is to clarify the difference created between the applied electric field and the mechanical strain. The actuators possess inherent forces such as strain and movement to accelerate the displacement process that occurs in strain and their derivatives.

TABLE 14.3 Different SMA Actuator Materials [75, 78, 79] ⏎

S. No.	Type	Alloy
1	Fe alloys	Fe–28–31–Pd, Fe–Pd–Ni, Fe-23–Pt, Fe–Ni–Co–Ti
2	Heusler	Ni2MnGa
3	NiTi-based alloys	NiTi, NiTiCu, NiTiPd, NiTiFe, NiTiNb, NiTiGa, NiTiCo
4	Cu-based alloys	CuZn, CuZnAl, CuAlNi, CuAlNiMn
5	Ag-based alloys	AgCd
6	Au-based alloys	AuCd
7	Co-based alloys	CoNiAl

14.4 SMAs IN AEROSPACE APPLICATIONS

SMAs actually provide new and novel solutions to aerospace industries, and in fact, these integrated SMAs [83, 84] will play a major role in future aerospace technology. SMAs inculcate new and compact structures into aerospace systems by adopting simplicity by reducing their volume and weight.

SMAs help to morph the structural features of planes by providing increased speed and roll control, reducing power consumption and chamber damage. These problems were rectified by adopting the SmartWing Program, as well as Smart and Aircraft and Marine Propulsion System Demonstration [85, 86], which were considered as important projects recognized by the Defense Advanced Research Projects Agency.

The most important features required in aircraft applications and numerous smart materials used in aerospace industries are given in Table 14.4.

To decrease the cost of aerospace industries most of the commercial airline and space exploration industries and defense requires smart materials to sustain their standards with less economy. To meet the aforementioned quality, the most robust and economically feasible smart materials are needed in the market. These materials are designed by varying their constitutions, by adopting special processing that includes rectifying the defects and modification of microstructures.

TABLE 14.4 Utility of Different Kinds of Smart Materials in Aerospace Industries [90] ⏎

S. No	Requirements	Materials	Purposes
1.	Design of smart materials for actuators for rotor control	Magneto-responsive materials	Cyclic and active control
2.	Control panel as extending to wings of aircraft	SMAs	To solve limits of aircraft wing design
3.	Shape-changing technology	Shape-altering smart materials	For military aircraft (Next to new generation aircraft)
4.	Shape-changing technology	SMAs	Engineering blending and stretching abilities in wings and hingeless system
5.	Shape-changing technology	Pizeoelectric	Engineering blending and stretching abilities in wings and hingeless system

In recent times, smart material-based load-bearing actuators in prescribed composite structures were adopted in aircraft wings and rotor blades were designed according to Liang et al. [87], Garner et al. [88], Jardine et al. [89] concepts.

The controlled or established nature of smart materials falls on wide applications in designing and manipulating helicopter rotor blade shapes. In recent times, Boeing has utilized smart material-based actuator rotor technology, which reduces vibrations by almost 80% and also improves the performance of flight. It also has the ability to control surfaces over airplane wings.

Smart materials also emphasize their importance in controlling and designing processes of actuators and sensors.

14.5 NANOTECHNOLOGY AND SMART MATERIALS

The influence of nanotechnology as a tool has elevated the performance of smart materials, enabling the design of materials in a highly advanced state. References [91–93] concluded that nanotechnology-enabled smart materials revealed excellent performance than their conventional counterpart. Smart materials in nano regime expose greater response to external stimuli, due to their high surface-to-volume ratio [94] able to sense minute changes in the environment even at very low magnitudes.

There are some advantages when smart materials exist in a nano regime [90] and some are as follows:

1. smart materials in nano regime, optimize the response of smart materials to complex external stimuli and able to adapt or manage to unexpected situations and conditions;
2. provides good functionality and control over the system;
3. influence on engineering and processing techniques;
4. helps to improve most of the health monitoring systems in a smart and advanced manner.

From the above points, it concludes that smart materials in the nano regime will open up multimodal applications in most of the industrial sectors like aerospace, automotive, mini actuators, robotics, microelectrochemical systems, and so on.

14.6 SMART MATERIALS AS MICROELECTROCHEMICAL SYSTEMS

The 20th-century transistor has been replaced by MEMs in the 21st century and helps to enable some of the discoveries such as silicon-based pressure sensors for monitoring exhaust emissions, fuel, and hydraulics in most of the automotive industries. MEMs are known as a combination of elements [94] of mechanical and electrical components, which convert one form of energy into another form. Devices made from MEMs are extremely small or consist of microchips. This miniature device usually contains common silicon substrates along with mechanical and electrical elements, and actuators. The purpose of MEMs is to directly react with the physical environment in an effective way. In general MEMs alone or with combinations of other sensors, MEMS are considered as promising platforms for robots [95, 96] to detect control forces, and slippage and also to find the distance between objects for effective dexterous manipulation. MEMs-based robotics sensors, being lightweight and taking very minimum space to occupy, can be integrated into robotics and able to sense even gripping and stiffness. The perspective of MEMs is their empowerment [97, 98] to engender systems and they are related to microactuators such as microsensors and microminiature motion systems (e.g., microrobots). Smart materials and MEMs used in various applications are shown in Figure 14.9.

MEMs as a smart material are applied in various fields including energy harvesting, atomizers, acoustic resonators (sensors and actuators), and flexible and stretchable devices. Categories of smart materials are summarized [100] in Figure 14.10.

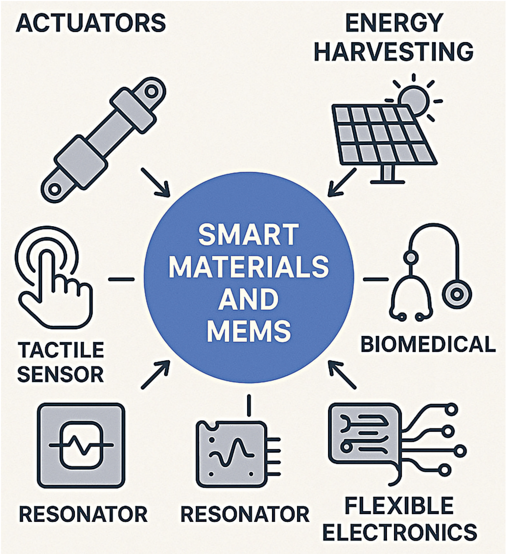
ACTUATORS
ENERGY HARVESTING
SMART MATERIALS AND MEMS
TACTILE SENSOR
BIOMEDICAL
RESONATOR
RESONATOR
FLEXIBLE ELECTRONICS

FIGURE 14.9 Smart materials and MEMs used in various applications [99]. ⏎

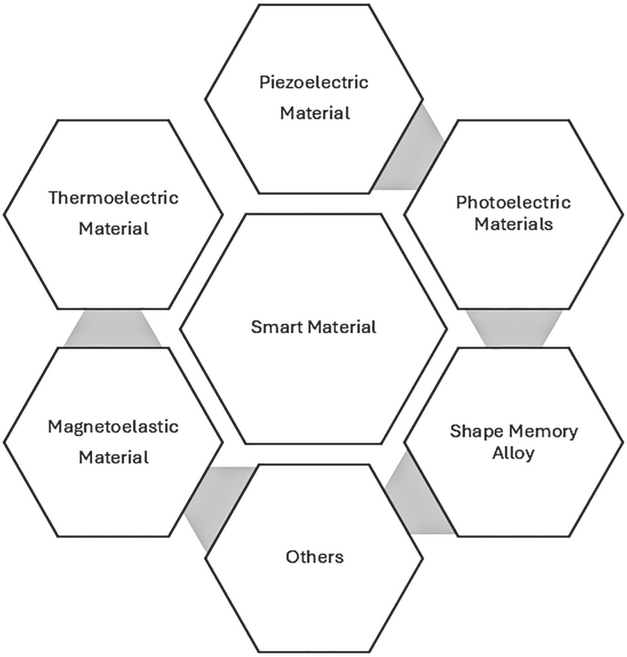
Piezoelectric Material
Thermoelectric Material
Photoelectric Materials
Smart Material
Magnetoelastic Material
Shape Memory Alloy
Others

FIGURE 14.10 Categories of smart materials [99]. ⏎

The smart sensors in MEMs help to communicate through feedback in closed-loop systems and are able to sense small changes in the environment and respond accordingly it changes its one or more of its property coefficients. By combining computing ability with sensing property, it has the propensity power to connect space and time with accuracy related to microlevel structure.

The interdisciplinary MEMs technology raises the development and fabrication of devices in various directions and in recent times many technologies adopt this smart mem with an integrated approach including mechanical, chemical, and biochemical sensors, and are marketed by different organizations.

14.7 CONCLUSIONS

To date, the most promising and flourishing technologies for the most reliable and lifetime efficiency include the utility of the most advanced materials like smart materials. To attain the full efficiency of these smart materials, one needs to understand the composition and ability to control the microstructure of these smart materials. The productivity of these smart materials inculcates the modern world's new dimensions such as, it reduces weight, eliminating sound, reflecting more light, and minimizing the size of most modern gadgets to robots and also in most aerospace parts. These smart materials provide an important impact on the respective surroundings as well as on the financial state. Hence, the proficiency of these smart materials helps to lead a quality life, like materials with environmental friendliness, and low-cost choices without changing materials efficiency, structural integrity, longevity, cost, and industrial probity is of utmost importance. New modern technologies were progressed in recent times to develop more advanced smart materials to offer more innovative solutions for unanswered problems in a long way.

KEYWORDS

- **smart materials**
- **smart memory alloy**
- **smart memory effect**
- **stimuli responsive materials and industrial applications**

REFERENCES

1. Murphy, E.B., Wudl, F. The world of smart healable materials. *Progr. Polym. Sci.*, **2010**, *35*, 223–251. https://doi.org/10.1016/j.progpolymsci.2009.10.006.
2. Takagi, T. A concept of intelligent materials and the current activities of intelligent materials in Japan. In *First European Conference on Smart Structures and Materials*, International Society for Optics and Photonics, 1992.
3. McCabe, J., et al. Smart materials in dentistry. *Aust. Dent. J.*, **2011**, *56*, 3–10.
4. Bogue, R. Smart materials: a review of recent developments. *Assembly Autom.*, **2012**, *32*(1), 3–7.
5. Hensel, M.U. Performance-oriented architecture and the spatial and material organisation complex. Rethinking the definition, role and performative capacity of the spatial and material boundaries of the built environment. *Form Akademisk for skning stids skrift for design og designdidaktikk*, **2011**, *4*(1).
6. Addington, D.M., Schodek, D.L. *Smart materials and new technologies: for the architecture and design professions*, Architectural Press, An imprint of Elsevier Linacre House: Jordan Hill, Oxford, 2005. ISBN 0 7506 6225 5.
7. Baumbick, R.J. Shape memory alloy actuator. In: US Patents 6151897. *The USA as represented by the Administrator of NASA*, Washington DC, USA. 2000, 7.
8. Sadeghi, M.J., Masudifar, P., Faizi, F. The function of smart material's behavior in architecture. In *International conference on intelligent building and management*. LACSIT Press, 2011.
9. Mohamed, A.S.Y. Smart materials innovative technologies in architecture; towards innovative design paradigm. *Energy. Procedia.*, **2017**, *115*, 139–154.
10. Song, Y., Wei, W., Qu, X. Colorimetric biosensing using smart materials. *Adv. Mater.*, **2011**, *23*(37), 4215–4236.
11. Clauser, H.R. Modern materials concepts make structure key to progress. *Mater. Eng.*, **1968**, *68*(6), 38–42.
12. Clauser, H.R. From static to dynamic materials in design. *Mech. Eng.*, **1975**, 20–26.
13. Historical developments and potential applications: smart materials and structures. 2016. http:/www.cambridge.org/core/terms. doi.org/10.1017/CBO9781139025164.002.
14. Savi, M.A., Steffen Jr, V.S. Special issue on smart materials and structures. *J. Braz. Soc. Mech. Sci. Eng.*, **2012**, *34*, 341–242.
15. Mishra, J. Smart materials—types SS and their application: a review. *Int. J. Mech. Produc. Eng.*, **2017**, *5*(12), 2320–2092.
16. Dye, D. Shape memory alloys: towards practical actuators. *Nat. Mater.*, **2015**, *14*(8), 760.
17. Bhuvaneshwari, S., Sasmal, B., Baskaran, S. Role of nano oxides for improving cementitious building materials. *J. Civ. Eng. Sci.*, **2012**, *1*(2), 52–58.
18. Ölander, A. An electrochemical investigation of solid cadmium-gold alloys. *J. Am. Chem. Soc.*, **1932**. *54*(10), 3819–3833.
19. Greninger, A.B., Mooradian, V.G. Strain transformation in metastable beta copper-zinc and beta copper-Ti alloys. *AIME Trans*, **1938**, *128*, 337–369.
20. Kumar, M.P., Simhachalam, D., Ramanaiah, N. A review on titanium niobium Shape Memory Alloys (SMA). *J. Mech. Eng. Sci.*, **2015**, 2293–9095.
21. Buehler, W.J., Wang, F.E. A summary of recent research on the Nitinol alloys and their potential application in ocean engineering. *Ocean. Eng.*, **1968**, *1*(1), 105–120.
22. Huang, W. Shape memory alloys and their application to actuators for deployable structures. 1998.

23. Hautcoeur, A., Fouché, F., Sicre, J. Cu-Al-Ni shape memory single crystal wires with high transformation temperature. In *43rd Aerospace Mechanisms Symposium*, 2016.
24. Smith, G. Photochromic glasses: properties and applications. *J. Mater. Sci.*, **1967**, *2*(2), 139–152.
25. Wu, M.H., Schetky, L.M. Industrial applications for shape memory alloys. In *International Conference on Shape Memory and Superelastic Technologies*. Pacific Grove: California, USA, 2000. pp 171–182.
26. Zider, R., Krumme J.F. Eyeglass frame including shapememory elements. In: US Patents 4772112. Menlo Park, California, USA: CVI/Beta Ventures, Inc.; 1988.
27. Hautcoeur, A., Eberthardt, A. Eyeglass frame with very high recoverable deformability. In *US Patents 5640217*. Fergaflex, Inc., Montreal, Canada, 1997.
28. Furuya, Y. Design and material evaluation of shape memory composites. *Intell. Mater. Syst. Struct.*, **1996**, *7*, 321–330.
29. Butera, F., Coda, A., Vergani, G. Shape memory actuators for automotive applications. In *Nanotec IT newsletter*. AIRI/nanotec IT: Roma, 2007. pp. 12–16.
30. Leo, D.J.,Weddle, C., Naganathan, G., Buckley, S.J. Vehicular applications of smart material systems. In *Proceedings of SPIE 3326, Smart Structures and Materials 1998: Industrial and Commercial Applications of Smart Structures Technologies*, 1998, pp. 106–116.
31. Stoeckel, D. Shape memory actuators for automotive applications. *Mater. Des.*, **1990**, *11*, 302–307.
32. Bil, C., Massey, K., Abdullah, E.J. Wing morphing control with shape memoryalloy actuators. *J. Intell. Mater. Syst. Struct.*, **2013**, *24*, 879–898.
33. Humbeeck, J.V. Non-medical applications of shape memory alloys. *Mater. Sci. Eng. A.*, **1999**, 134–148
34. McDonald Schetky, L. Shape memory alloy applications in space systems. *Mater. Des.*, **1991**, *12*, 29–32.
35. Kohl, M. *Shape memory microactuators (microtechnology and MEMS)*. 1st edn. Springer-Verlag, Berlin: Heidelberg, 2010.
36. Sun, L., Huang, W.M., Ding, Z., Zhao, Y., Wang, C.C., Purnawali, H., et al. Stimulus responsive shape memory materials: a review. *Mater. Des.*, **2012**, *33*, 577–640.
37. Cederström, J., Van Humbeeck, J. Relationship between shape memorymaterial properties and applications. *J. Phys. IV France.*, **1995**, *05*, C2-335–C2-341.
38. Wilkes, K., Liaw, P., Wilkes, K. The fatigue behavior of shape memory alloys. *JOM*, **2000**, *52*, 45–51.
39. Hodgson, D.E., Wu, M.H., Biermann, R.J. Shape memory alloys. ASM Handbook. *ASM International*, **1990**, 897–902.
40. Huang, W. On the selection of shape memory alloys for actuators. *Mater. Des.*, **2002**, *23*, 11–19.
41. Sun, L., Huang, W.M. Nature of the multistage transformation in shape memory Alloys upon heating. *Met. Sci. Heat. Treat.*, **2009**, *51*, 573–578.
42. Mihálcz, I. Fundamental characteristics and design method for nickeltitanium shape memory alloy. *Periodica. Polytechnica. Ser. Mech. Eng.*, **2001**, *45*, 75–86.
43. Jani, J.M., et al. A review of shape memory alloy research, applications and opportunities. *Mater. Des.*, **2014**, *56*, 1078–1113.
44. Lagoudas, D.C. *Shape memory alloys: modeling and engineering applications*. 1st edn. Springer: New York, 2010.
45. Duerig, T.W., Pelton, A.R. *Ti–Ni shape memory alloys. materials properties handbook, titanium alloys*. American Society for Metals: Materials Park, OH, **1994**, pp. 1035–1048.

46. Mishra, J., Singh, T. Shape memory alloys and their potential application: a review. *Int. J. Curr. Res.*, **2017**, *9*(10), 59186–59192.
47. Boyn, S., Grollier, J., Lecerf, G., et al. Learning through ferroelectric domain dynamics in solid-state synapses. *Nat. Commun.*, **2017**, *8*, 1–7.
48. Sharma, K., Srinivas, G. Flying smart: smart materials used in aviation industry. *Mater. Today: Proc.*, **2019**, https://doi.org/10.1016/j.matpr.2019.10.115.
49. Drossel, W.G., H. Kunze, A., Bucht, L., Pagel, K. Smart3–Smart materials for smart applications. *Procedia CIRP*, **2015**, *36*, 211–216.
50. Sot, R., Kurzydlowski, K.J. Ab initio calculations of elastic properties of Ni3Al and TiAl under pressure. *Mater. Sci.-Pol.*, **2005**, *23*(3), 587–590.
51. Hosoda, Y. Application of shape memory alloy for robots. *JSME Semin.*, **1987**, *53*, 648.
52. Mândru, D., et al. *Actuating systems in precision engineering and mechatronics*, Alma Mater: Cluj-Napoca, 2004.
53. Luchetti, T., Zanella, A., Biasiotto, M., Saccagno, A. Electrically actuated antiglare rear-view mirror based on a shape memory alloy actuator. *J. Mater. Eng. Perform.*, **2009**, *18*, 717–724.
54. Manzo, J., Garcia, E., Wickenheiser, A., Horner, G.C. Design of a shape-memory alloy actuated macro-scale morphing aircraft mechanism. In *Proceedings of SPIE 5764, Smart Structures and Materials 2005: Smart Structures and Integrated Systems,* 2005, pp. 232–240.
55. Johnson, R.W., Evans, J.L., Jacobsen, P., Thompson, J.R., Christopher, M. The changing automotive environment: high-temperature electronics. *IEEE Trans. Electron. Pack. Manuf.*, **2004**, *27*, 164–176.
56. Stoeckel, D. Shape memory actuators for automotive applications. *Mater. Des.*, **1990**, *11*, 302–307.
57. Shrikant, K.Y., Rupesh, S.B. Shape memory alloy actuators: a review. *Int. J. Res. Appl. Sci. Eng. Technol.*, **2019**, *7*(5), 2321–9653. https://doi.org/10.22214/ijraset.2019.5134.
58. William, L., Benard, H.K., Arthur, H., Heuer., Michael, A.H. Thin-film shape-memory alloy actuated micropumps. *J. Micro. Electromech. Sys.*, **1998**, *7*(92), 245–251.
59. Johnson, A.D., Busch, J.D., Ray, C.A., Sloan, C.L. Fabrication of silicon-based shape memory alloy micro actuators. *Mater. Res. Soc. Symp. Proc.*, **1992**, *276*, 151–160.
60. Ikut, K., Tsukumoto, M., Hirose, S. In Shape memory alloy servo actuator system with electric resistance feedback and application for active endoscop. In *IEEE*, 1988.
61. Peng, F., Jiang, X.X., Hu, Y.R. Application of shape memory alloy actuators in active shape control of inflatable space structures. In *IEEE*, 2004. 8, 1–10.
62. Balta, J.A., Simpson, J., Michaud, V., Månson, J.A.E., Schrooten, J. Embedded shape memory alloys confer aerodynamic profile adaptivity. *Smart. Mater. Bull.*, **2001**, 8–12.
63. Williams, E.A., Shaw., Elahinia, M. Control of an automotive shape memory alloy mirror actuator. *Mechatronics*, **2010**, *20*, 527–534.
64. Jani, J.M., Leary, M., Scbic, A., Mark, A. A review of shape change memory alloy research, applications and opportunities, Elsevier. *J. Mater. Des.*, **2014**, *56*, 1078–1113.
65. Bogue, R. Shape-memory materials: a review of technology and applications. *Assembly. Autom.*, **2009**, *29*, 214–219.
66. Luchetti, T., Zanella, A., Biasiotto, M., Saccagno, A. Electrically actuated antiglare rear-view mirror based on a shape memory alloy actuator. *J. Mater. Eng. Perform.*, **2009**, *18*, 717–724.

67. Manzo, J., Garcia, E., Wickenheiser, A., Horner, G.C. Design of a shape-memory alloy actuated macro-scale morphing aircraft mechanism. In *Proceedings of SPIE 5764, Smart Structures and Materials 2005: Smart Structures and Integrated Systems,* 2005, pp. 232–240.
68. Williams, E., Elahinia, M.H. An automotive SMA mirror actuator: modeling, design and experimental evaluation. *J. Intell. Mater. Syst. Struct*., **2008**, *19*(12), 1425–434.
69. Mândru, D., Lungu, I., Noveanu, S., Tătar, O. Applications of shape memory alloy actuators in biomedical engineering. *Fascicle of Management and Technological Engineering*, **2008**, *VII*(XVII), 922–927.
70. Mikova, Ľ., Medvecka, S. Application of shape memory alloy (sma) as actuator. *Metalurgija*, **2015**, *541*, 169–172.
71. Bidaud, P.R.I., Collard, D., Buchaillot, L. Fabrication and characterization of an SU-8 gripper actuated by a shape memory alloy thin film. *J. Micromech. Micr. Eng*., **2003**, *13*(2), 330.
72. Ming, H., Wu, L., Schetky, M.C.D. Industrial applications for shape memory alloys. In *Proceedings of the International Conference on Shape Memory and Superelastic Technolgies*, California: Pacific Grove, 2000, pp. 171–182.
73. Stoeckel, D., Waram, T. Use of Ni–Ti shape memory alloys for thermal sensor actuators. In *Active and adaptive optical components*, SPIE: San Diego, CA, 1992, pp. 382–387.
74. Peirs, J. A micro robotic arm for self propelling colonoscope. In *Proceedings of the 6th International Conference on New Actuators Actuator*, 1998, Vol. 98, pp. 576–579.
75. Taya, M., Kato, H. Development of ferromagnetic shape alloys based on FePd alloy. In *Proceedings of the Asian Pacific Conference on Fracture and Strength and International Conference on Advanced Technology in Experimental Mechanics*, 2001, pp. 11–20.
76. Novac, A., Sprincenatu, R. Martensitic transformation in Fe-Pd ferromagnetic shape memory alloy wires. In *7th International Conference on Advanced Materials and Structures*, 2018, pp. 1–5.
77. Mielke, T., Maris, J., Gopfert, W., Murrenhoff, H. Potential of ferromagnetic shape memory alloys as power units in hydraulic pumps. In 2018 Global Fluid Power Society PhD Symposium (GFPS), IEEE, 978-1-5386-4785-1/18.
78. Huan, W. Shape memory alloys and their application to actuators for deployable structures. PhD Thesis, Cambridge University. 1998.
79. Ölander, A. An electrochemical investigation of solid cadmium-gold alloys. *Am. Chem. Soc*., **1932**, *54*, 3819–833.
80. Lagoudas, D.C., Garner, L.J., Rediniotis, O.K., Wilson, N. Modeling and experiments of the hysteretic response of a active hydrofoil actuated by SMA line actuators. *Smart structures*, Kluwer Academic Publisher: Dordrecht, 1999, pp. 153–162.
81. Dosch, J.J., Inman, D.J., Garcia, E. A self-sensing piezoelectric actuator for collocated control. *J. Intell. Mater. Syst. Struct.*, **1992**, *3*, 166–185.
82. Gupta,V., Sharma, M., Thakur, N. Optimization criteria for optimal placement of piezoelectric sensors and actuators on a smart structure: a technical review. *J. Intell. Mater. Syst. Struct.*, **2010**, *21*(12), 1227–1243.
83. Costanza, G., Tata, M.E., Calisti, C. Nitinol one-way shape memory springs: thermomechanical characterization and actuator design. *Sens. Actuator. A. Phys*., **2010**, *157*, 113–117. https://doi.org/10.1016/j.sna.2009.11.008.

84. Costanza, G., Paoloni, S., Tata, M.E. IR thermography and resistivity investigations on Ni-Ti shape memory alloy. *Key. Eng. Mat.*, **2014**, *605*, 23–26. https://doi.org/10.4028/www.scientific.net/KEM.605.23.
85. Garcia, E. Smart structures and actuators: past, present, and future. In *Proceedings of the SPIE Smart Structures and Materials,* San Diego, CA, USA, 2002, Vol. 27, pp. 1–12.
86. Sanders, B., Crowe, R., Garcia, E. Defence advanced research projects agency—Smart materials and structures demonstration program overview. *J. Intell. Mater. Syst. Struct.*, **2004**, *15*, 227–233. https://doi.org/10.1177/1045389X04042793.
87. Liang, C., Davidson, F., Schetky, L.M., Straub, F.K. Applications of torsional shape memory alloy actuators for active rotor blade control-opportunities and limitations. In *SPIE Proceedings of Mathematics and Controls in Smart Structures*, 1996, 2717, pp. 91–100.
88. Garner, L.J., Wilson, L.N., Lagoudas, D.C., Rediniotis, O.K. Development of a shape memory alloy actuated biomimetic vehicle. *Smart. Mater. Struct.*, **1999**, *9*, 673–683.
89. Jardine, A.P., Kudva, J.M., Martin, C., Appa, K. Shape memory alloy Ti-Ni actuators for twist control of smart wing designs. In *SPIE Proceedings of Mathematics and Controls in Smart Structures*, 1996, 2717, pp. 160–165.
90. Basheer, A.A. Advances in the smart materials applications in the aerospace industries. In *Aircraft engineering and aerospace technology*, Emerald Publishing Limited. 2020, Vol. 92/7, pp. 1027–1035 [ISSN 1748-8842], https://doi.org/10.1108/AEAT-02-2020-0040.
91. Ali, I. New generation adsorbents for water treatment. *Chem. Rev.*, **2012**, *112*, 5073–5091.
92. Ali, I. Microwave-assisted the economic synthesis of multi-walled carbon nanotubes for arsenic species removal in water: batch and column operations. *J. Mol. Liq.*, **2018**, *271*, 677–682.
93. Coyle, S., Wu, Y., Lau, K.D. Smart nano-textiles: a review of materials and applications. *MRS Bulletin*, **2007**, *32*(5), 434–442.
94. Dahman, Y., Kamil, A., Baena, D. Smart nanomaterials. In Dahman, Y. (Ed.), *Nanotechnology and functional materials for engineers*. Elsevier, 2017.
95. Jackson, N., O'Murchu, C., Mathewson, A., Olszewski, O. Powering a leadless pacemaker using a PiezoMEMS energy harvester. *SPIE Microtechnologies*, **2017**, 102460V.
96. Olszewski, O., Houlihan, R. A MEMS silicon-based piezoelectric AC current sensor. *Eurosensors*, **2014**, *87*, 1457–1460.
97. Jackson, N., Keeney, L., Mathewson, A. Flexible aluminium nitride/polyimide piezoelectric material for MEMS applications. In *The 10th International Workshop on Piezoelectric Materials and Applications in Actuators (IWPMA) and 8th Annual Energy Harvesting Workshop (EHW)*, Hannover, Germany, 2013.
98. O'Keeffe, R., Jackson, N., O'Neill, M., McCarthy, K., Mathewson, A. Investigation into modelling power output for MEMS energy harvesting devices using COMSOL multiphysics. In *IEEE Conference on Thermal, Mechanical, and Multi-Physics Simulation and Experiments with MEMS*, Wroclaw, Poland, 2013.
99. Jackson, N.J., Pedrosa, J., Bollero, A., Mathewson, A., Olszewski, O. Integration of thick permanent magnets for MEMS applications. *IEEE J. Microelectromech. Syst.*, **2016**, *25*(4), 716–724.
100. Pinheiro, E.D., Deivarajan, T. A concise review encircling lead free porous piezoelectric ceramics. *Acta. Physica. Polonica. A.*, **2019**, *136*, 555–565. https://doi.org/10.12693/APhysPolA.136.555.

CHAPTER 15

IMPACT OF MATERIALS IN SOLAR PHOTOVOLTAIC APPLICATIONS IN STANDALONE SYSTEM

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ABSTRACT

This chapter outlines the emerging solar photovoltaic applications, its benefits, classification of solar PV materials, and its usage in the solar power generation. Some logical concepts related to maximum power point tracking are presented and various topologies of inverters are briefly discussed. Need of an inverter is must for solar PV system, so various types of inverters with their flow diagram, advantages, disadvantages, and its basic comparison stating which one would be best for use is also mentioned briefly.

15.1 INTRODUCTION

Solar energy is preferred over other nonconventional sources due to its eco-friendliness and other benefits, as well as the fact that it is pollution-free, infinite, and requires less upkeep [1]. In the current scenario, the concept of standalone solar photovoltaic system is becoming popular, as it benefits people, living far away from the utility grid and are dependent on it for their daily running appliances at home or business [2].

The rooftop PV panels are manufactured using monocrystalline, polycrystalline, or amorphous silicon panels [3]. The main criterion of the system is to take upon maximum illumination at different radiation conditions [4]. Certain areas are affected by inconsistent solar radiation, which requires a battery storage. So different methods like bulk charging, absorption charging, and float charging are used [5]. Also, the remote areas, which are affected by the transmission of electricity, need a proper attention with the help of standalone solar photovoltaics. To increase the green energy generation, a hybrid arrangement [6] is best suitable as per the calculations and simulations in [7]. Along with this, an Integrated system of PV panels is discussed in [8] as a benefit to residential areas.

Residential load varies but continuous power supply is required. For this, the type, size, and the operational sequence of solar PV are required [9]. Also, the cost of batteries needs to be reduced by making their size miniaturized and if capital cost of PV system reduces [10], it acts as an add on factor.

15.2 STANDALONE SOLAR PHOTOVOLTAICS

Figure 15.1 shows the simplified schematic diagram of standalone solar photovoltaic.

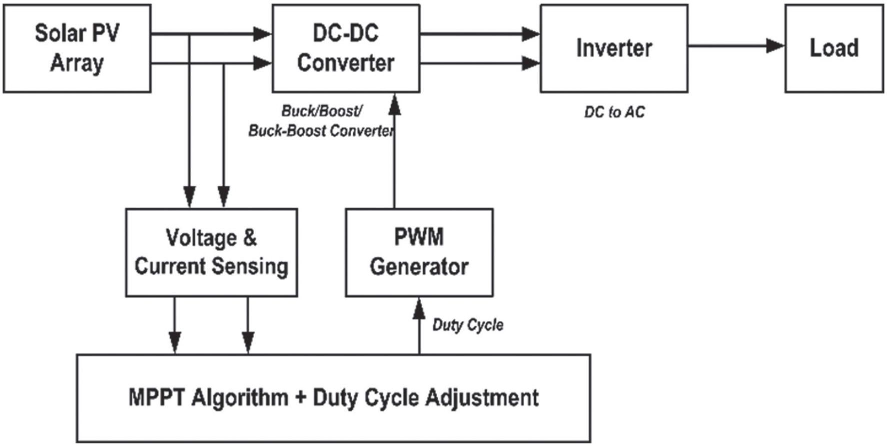
Solar PV Array
DC-DC Converter
Buck/Boost/ Buck-Boost Converter
Inverter
DC to AC
Load
Voltage & Current Sensing
PWM Generator
Duty Cycle
MPPT Algorithm + Duty Cycle Adjustment

FIGURE 15.1 Simplified solar photovoltaic system. ⏎

Regardless of temperature, solar irradiation, and various load situations, the concept of maximum power point tracking (MPPT) is applied to harvest the most energy from the solar panels. It is used as a procedure to withdraw maximum available energy from the solar modules by varying the converter's duty cycle in such a manner that the operating point is constantly pushed in response to increasing power [11]. As shown in Figure 15.1, the input voltage to the DC–DC converter is adjusted using the pulse width modulation (PWM) approach. For the PWM technique, a control strategy of voltage–frequency (v–f) can also be used [12]. For an optimal functioning, various studies of different characteristics of the solar modules is to be done, so that the optimal operation with various loads can be tackled [13].

The configuration of the standalone system consists of PV panels, charge controllers, storage devices, and inverters for the AC supply to the loads [14]. Often the open loop output outcomes are to be checked with the experimental outcomes to look and verify the efficiency of results [15]. In certain advancements, LED driving circuit with the PV system is given [16] where primary current source is the solar PV panels and bi-directional converter incorporated to the battery behaves as an auxiliary current source.

15.3 CONCEPT OF MPPT AND ITS ALGORITHM

In solar-powered modules, there is only one working point from which the maximum power can be extracted at any given time. The first step is to locate and keep an eye on this point to make sure that the maximum power point tracking (MPPT) module's operating point is constantly there or nearby. Therefore, the MPPT concept refers to the strategy of constantly keeping the operational point of the solar module at the most optimal available location of the power spot.

It aims to boost the system's overall performance [17]. As shown in Figure 15.2, which is the general IV characteristic of PV cell, here we can evaluate the maximum power point (MPP), where $P_{\text{mpp}} = V_{\text{mpp}} I_{\text{mpp}}$

The slope of the line depends on the impedance of the load when the dotted line is used as the load line. So, if the slope decreases, impedance value increases and vice-versa. So different algorithms are required for the MPPT technique. Mainly two techniques are used as follows:

The Perturb and Observe (P&O) method involves the addition of a perturbation or divergence. As a result, the power of the solar modules is continuously changed. The direction of further increases in disturbance is typically the same. The power at the following step decreases after reaching its peak, which causes the divergence to reverse. This algorithm drifts in and out of the steady state as it approaches the peak. The conventional P&O approach is improved by the fractional short-circuit current method [18].

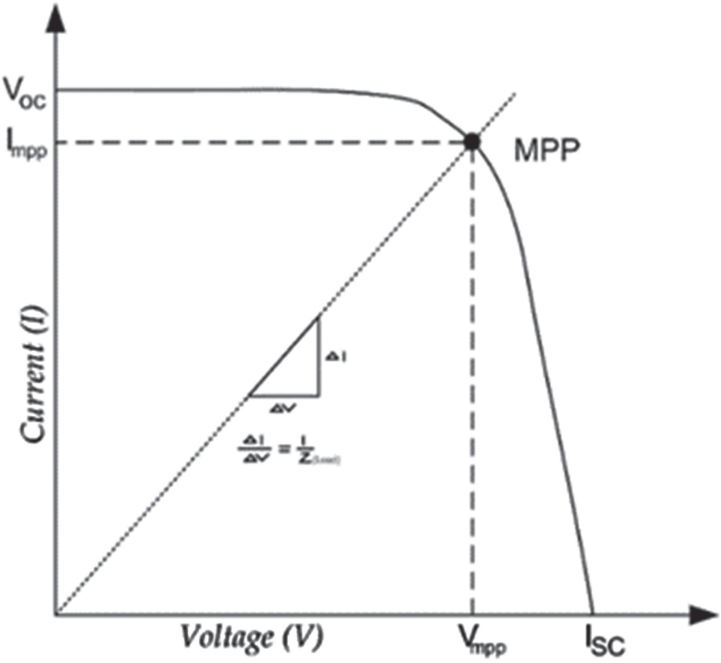

FIGURE 15.2 I–V characteristics of PV cell. ⏎

P&O approach provides accurate results in typical weather conditions, however when the climate changes, the MPPT algorithm is designed using an artificial neutral network [19]. Voltage is used as a reference and control parameter in voltage perturbation, and duty ratio is used as a control parameter in duty ratio perturbation [20]. Basically, the power and the voltage elements are crucial in P&O algorithm.

Using the incremental conductance method, the general P&O algorithm's defect is fixed. This algorithm tracks the MPP under varied environmental conditions. By using this technique, it is certain that the tracker will end running at the operational point where its power is at its peak [21]. The value of the differential power to differential voltage ratio is negative and positive, respectively, when the tracker is to the right of the maximal power point and to the left [22]. As a result, when P&O maneuvers around MPP, the IC algorithm determines the MPP. This shows the clear advantage of the latter. The procedure can be easily understood from Figure 15.3.

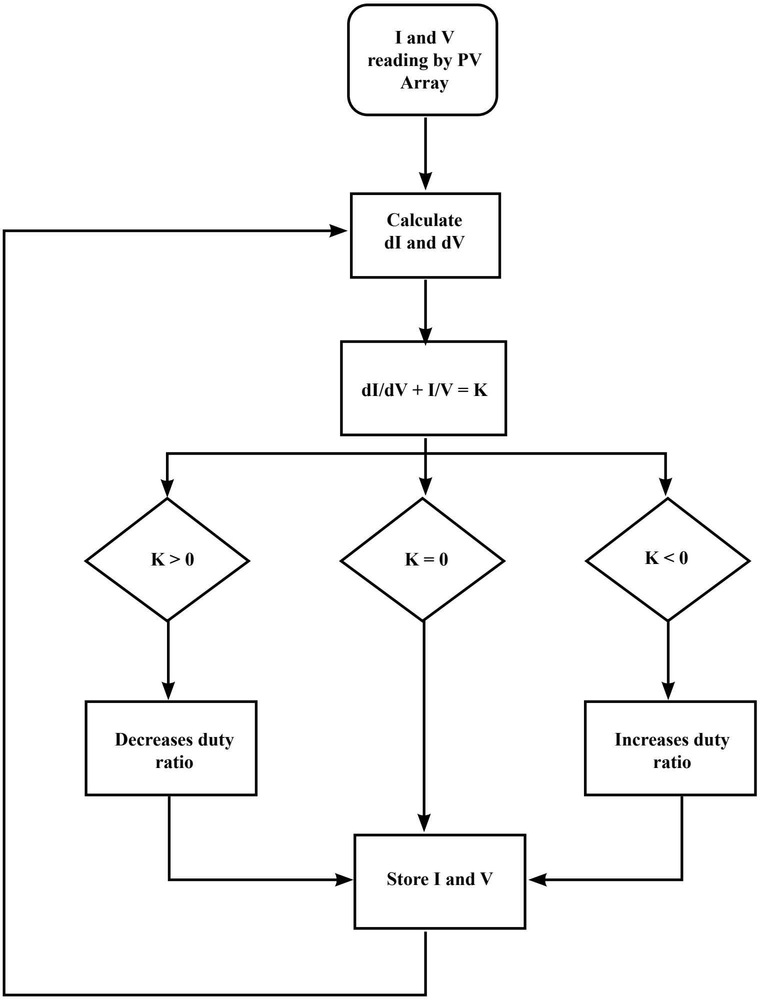
I and V reading by PV Array
Calculate dI and dV
dI/dV + I/V = K
K > 0
K = 0
K < 0
Decreases duty ratio
Increases duty ratio
Store I and V

FIGURE 15.3 Incremental conductance flow diagram. ⏎

IC algorithm improves the stable-state performance and quick reaction of the PV system [23]. IC is more efficient than P&O method as it is stable under steady-state conditions because it measures all voltages and currents of PV system at every instant of time, while P&O measures in periodic power [24]. Different readings of voltages and currents in different conditions like in a cloudy or sunny day are taken [25]. Also, under partial shading, multivariable particle swarm optimization technique [26] and the steepest descent MPPT algorithm are mentioned in [27]. Various strategies of MPPT are discussed in [28] where an improvement by 2% is observed by certain variable step and predicts current control system. Efficiency of MPPT is increased by using automatic selection of algorithm (ASA) with help of ASA switches [29]. Variations in algorithms is seen where the PV system uses a single sensor neutral network MPPT controller to track maximum power [30]. Combination of these methods is also observed in [31]. PV inverter MPPT's evaluation index is used to test the efficiency of it [32].

Nowadays new intelligent processing methods and nonlinear restraining strategies are used like fuzzy logic algorithm [33]. The fuzzy logic algorithm requires more readings as compared to P&O. Although it achieves precise values for any irradiation and temperature [34]. Also, it has less rippling than P&O [35]. MPPT is designed to operate under any condition. MPPT and non-MPPT outputs are compared using simulation [36].

15.4 DC–DC CONVERTER

DC–DC converters are employed when an average output voltage that can be compared to an input voltage that is higher or lower in magnitude is needed. These converters come in three topologies: The three converters are Buck Converter ($V_{in}>V_{op}$), boost converter ($V_{in}<V_{op}$), and buck–boost converter. The buck converter is a chopper whose output voltage is lower when compared to input voltage but whose output current is higher than input (Figures 15.4 and 15.5).

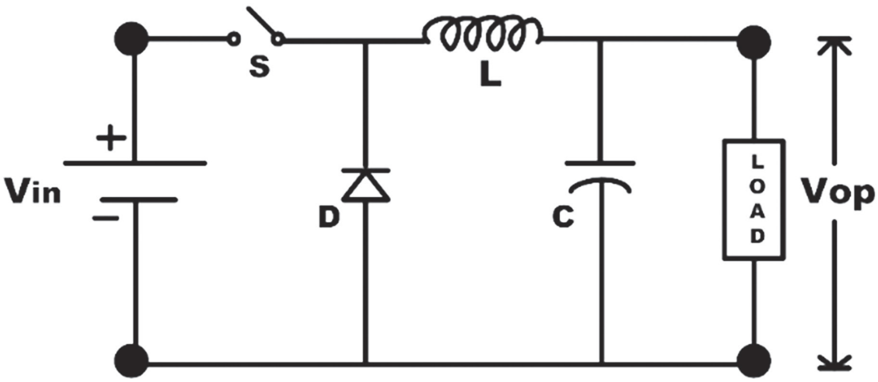

FIGURE 15.4 Buck converter. ⏎

The conversion ratio can be indicated by

$$V_{op} / V_{in} = D \text{ (Duty ratio)} \tag{15.1}$$

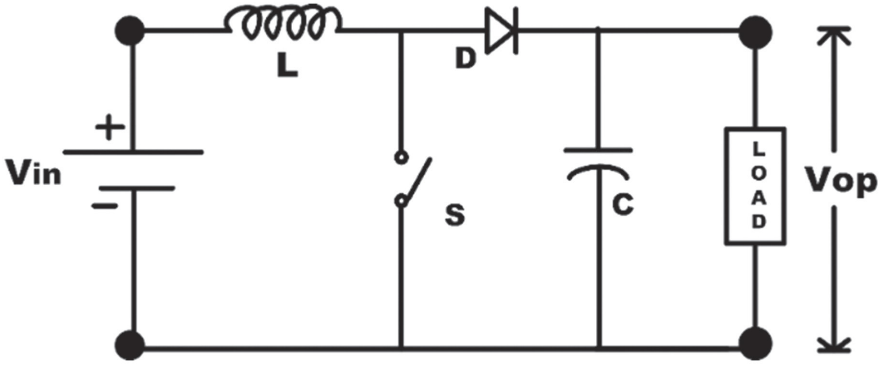

FIGURE 15.5 Boost converter. ⏎

$$\text{So, by the above expression, } V_{in} = V_{op}/D \tag{15.2}$$

Boost converter: Although the output current of this converter is lower than the input current, the output voltage is higher than the input voltage.

The conversion ratio can be indicated by

$$V_{op} / V_{in} = 1/(1-D) \text{ (Duty ratio)} \tag{15.3}$$

$$\text{So, by the above expression, } V_{in} = V_{op}\,(1-D) \tag{15.4}$$

The energy storage function of the inductor (L) is useful for the operation of the converter. Also, the switch (S) can be taken as MOSFET where the gate pulse has an input from the PWM. The diode (D) connected works as a freewheeling diode.

These converters can be connected in series or parallel connection [37]. In order to lessen switching stress, boost converters are utilized in continuous conduction mode [38]. Also, voltage at input side is less and current at output side is more, circuit resistance needs to be maintained. Push–pull type arrangements are thought of by controlling the point at which maximum power is achieved [39]. A continuous low ripple input current is most desired which is a must requirement for MPPT also. The analysis of the output is carried out in steady-state condition [40]. The disadvantages of the general boost converter are high stress voltage and high peak current for power devices which can be overcome by using interleaved converter [41]. There are various ways to increase the gain a high output at the end of DC–DC converter such as by using a diode-capacitor-based single-ended primary-inductor converter chopper with a voltage multiplier cell method reduces the voltage stress and rise in more voltage gain [42]. These converters need to increase the voltage magnificently with a bearable cost of reduced efficiency. So, in [43] a two-stage conversion is mentioned. A three-level DC–DC boost converter attached with the solar panels along with isolated bidirectional converter is preferred in [44] for rooftop PVs.

A PWM-based strategy of two-loop PI control may be used to manage the magnitude of voltage obtained at the bus load in the context of a persistent power load in a solar battery standalone direct current system. Here the inductor current is controlled with the help of inner loop whereas the voltage at load bus is controlled by outer loop. Instant maximum power is extracted from solar panel by IC method using a step-up converter irradiation and varying load conditions [45]. Solar photovoltaic charger uses a current-controlled converter for purpose of charging a high-volume battery bank [46]. A power flow management system can also be used for a solar panel distribution, by using a sole stage inductor-based dual output/input converter feeding a stand-alone DC load, supported by a rechargeable battery [47]. A bi-directional port is also connected to the storage system, and the output terminal is connected to the load [48]. Shut-down mode along with buck and boost mode can be seen in [49]. Dual input converters are an option as well, where dual inputs refer to a solar PV source and an ideal DC source, respectively. This particular inverter may accept input from both sources simultaneously or sequentially [50]. A unique circuit consisting of one coupled inductor and three capacitors is given in [51]. Here, the unique circuit makes it possible for both high gain and high efficiency. For buck–boost-type converters, the inductor should be chosen which ensures that saturation current is larger than inductor apex current and is capable to match up with the rms current [52]. With this, CUK converters are also preferred [53].

After the gain or reduction in voltage, the new DC output is fed to the inverter for DC-AC conversion. Loads are in requirement of AC supply needs a highly efficient inverter.

15.5 INVERTER AND TOPOLOGIES

Inverter converts the DC to AC with some topologies as discussed. Multilevel inverter topologies are:

Multilevel Inverter (MLI): MLI has more advantages if equated to these 2-level inverters; it can operate on several voltages, minimal harmonic perversion reduced EMI/EMC generation. The purpose of MLI is to use high power with the help of using series of semiconductor switches [54]. The rating of this switch depends on capacity of voltage sources to which they are connected [55]. There are many advantages of MLI, which includes reducing the dV/dT stress, EMC is also reduced and it also draws input current at low distortion. They also have some drawbacks, such as a large number of semiconductor switches that impact the system's overall performance and make it costly and complex [56]. Various industries have now started using applications that requires enormous amount of power. Due to their use as a substitute in scenarios requiring medium voltage and high power, multilevel inverters have attracted enormous demand from the power sector. Hence in this chapter, a detailed discussion of various multilevel inverter topologies along with their advantages and drawbacks and the application part are discussed. Multilevel inverters are broadly classified into two parts [57]:

1. Single DC source
2. Separate DC source

15.5.1 DIODE-CLAMPED MULTILEVEL INVERTER (DCMLI)

By clamping the voltage with diodes, this sort of architecture aims to lessen the voltage stress on power components. In this case, inverter diodes are employed to assist in supplying varied voltage levels to capacitor banks that are collectively connected in a series connection as seen in Figure 15.6 through various phases. The highest output voltage in this case, like in Figure 15.6, is equal to the input voltage divided by two.

The three-level diode clamped multilevel inverter shown in the above image has S1, S2, S1', and S2' acting as switches and parallel diode, D1 and D2 acting as clamp diodes, and C1 and C2 acting as series capacitor banks. The general approach to calculating the number of components in the inverter is shown in Table 15.1.

Single DC source includes diode clamp and flying capacitor inverters whereas separated DC source includes H-bridge cascaded inverters.

15.5.2 FLYING CAPACITOR INVERTER (FCI)

The main distinction between the operation of this kind of inverter and a diode-clamped inverter is the use of capacitors rather than diodes for clamping.

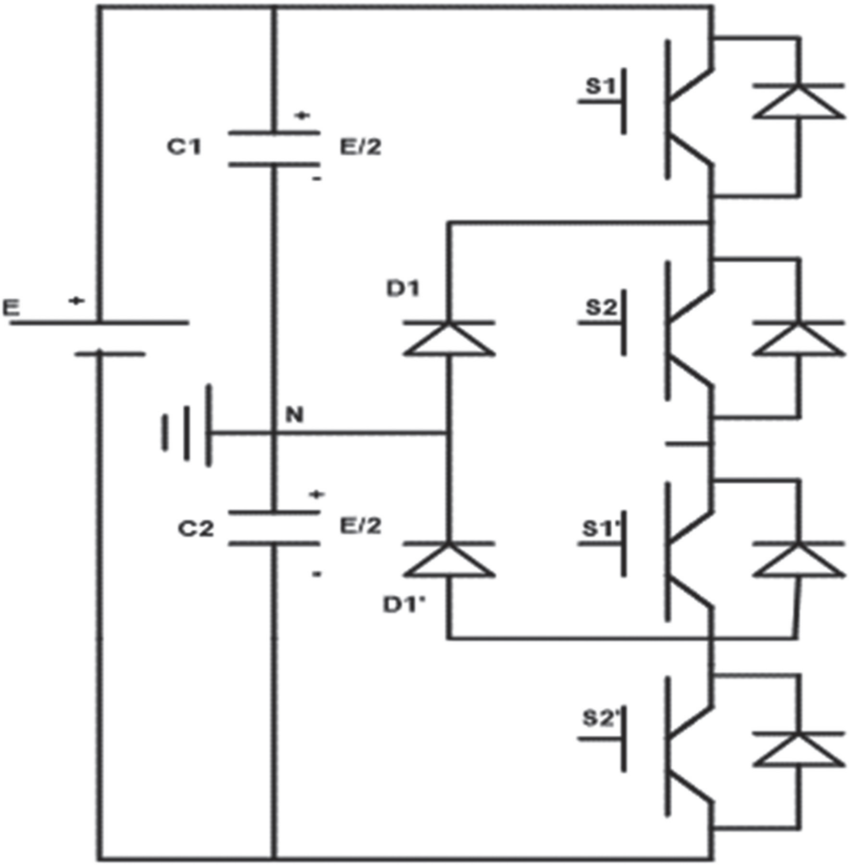

FIGURE 15.6 DCMLI. ⏎

TABLE 15.1 Diode Clamped Inverter Number of Components ⏎

Sr. No.	Name	General	Fig 1 (K=3)
1	Levels	K	3
2	Switches and Parallel Diodes	2K-2	4
3	Capacitors	K-1	2
4	Clamp Diodes	(K-1)* (K-2)	2

As we can see in Figure 15.7, the only change in flying capacitor MLI is that diodes D1 and D1′ are replaced by C3. The capacitor transfers limited amount of power to electrical device as it has power storing capability.

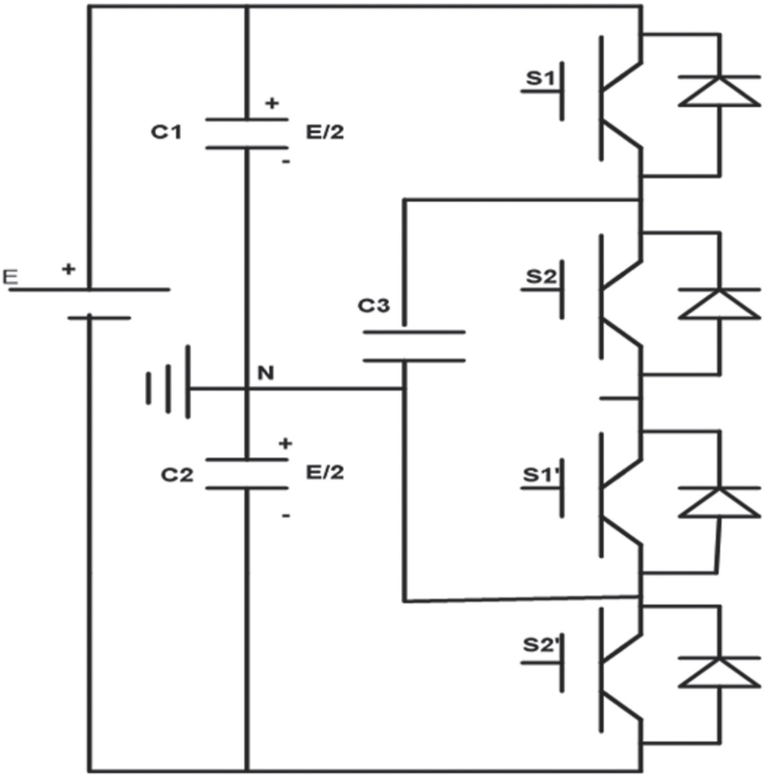

FIGURE 15.7 FCI. ⏎

Advantages

1) The problem of voltage sharing faced by diode clamped is rectified by this type of inverter.
2) Capacitors provide a huge amount of storage and hence less load to connected devices.

Disadvantages

1) As the number of level increases number of capacitors also increase.

Application

1) Control of induction motor
2) As sinusoidal current rectifier
3) Static Var generation.

15.5.3 H-BRIDGE-BASED CASCADED MULTI-LEVEL INVERTER (HBCMLI)

One of the special reasons to use this type of inverters is that it requires a few numbers of switches as compared to multilevel inverter, and it uses more than one type of DC source and the summation of all levels at which voltage is produced by each of the cell is equal to the output voltage. They are considered as one of the best for PV grid-connected applications since various sources are needed on the DC side. As the levels in an inverter are seen increasing, the harmonic distortion is experienced less amount [58, 59] (Figure 15.8).

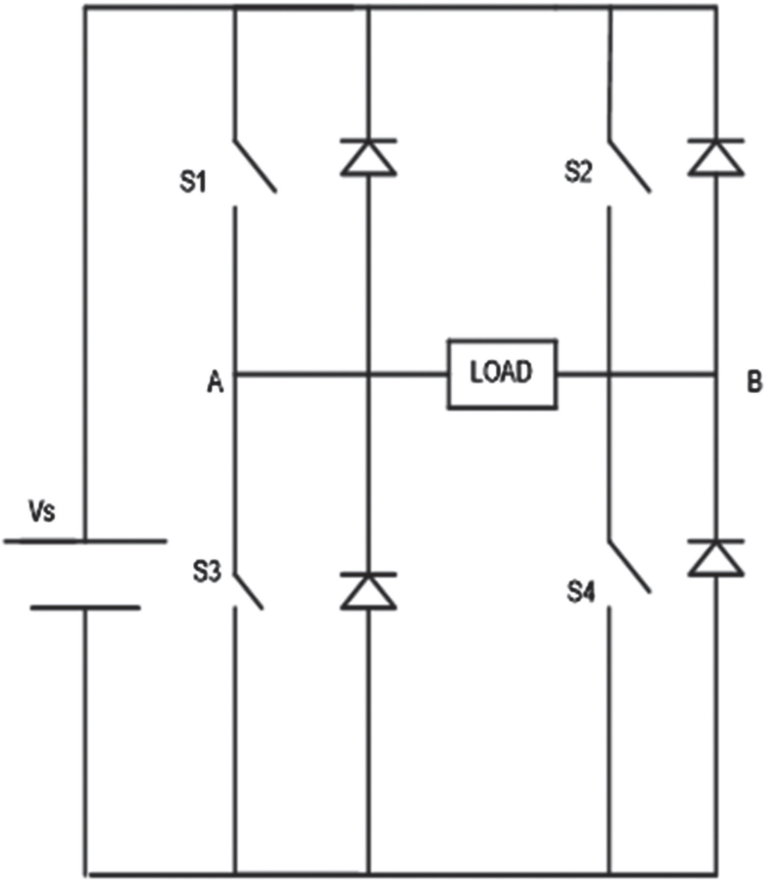

FIGURE 15.8 HBCMLI. ⏎

Advantages

1) In this type of inverter, initial capacitor charging and balancing problems are eliminated [59].
2) Total harmonic distortion (THD) decreases drastically since levels in the inverter are increased.

Disadvantages

1) Number of DC sources increases when we increase the level.
2) Complex control of the circuit because of more elements.

Application

1) Power factor compensator
2) Electric vehicle drives

15.6 SOLAR PV MATERIALS

The discovery of P–N junction solar cell in 1954 has led to many new inventions in solar cell materials ever since.

Three categories are frequently used to group solar cell technologies: (1) First generation (1G) wafer-based silicon crystalline that includes monocrystalline and multi-crystalline silicon solar cells. (2) Second-generation (2G) solar cells include thin film solar cell (TFSC) in which amorphous-silicon (a-Si) solar cell, cadmium telluride (CdTe) and copper indium gallium di-selenide (CIGS) are the most commonly used materials. (3) Third-generation (3G) solar cell materials include relatively newer solar cell technologies mostly under testing and investigations in laboratories. The two most crucial elements for solar cell materials technology are efficiency and production cost. Devices made using first-generation (1G) solar cells have a decent efficiency but significant production costs. Second-generation TFSCs have lower efficiency than first-generation TFSCs, but they are less expensive to make. In order to attain reduced production costs and improved efficiency, the third generation of solar cells is hence the focus [60].

15.6.1 FIRST-GENERATION (1G) SOLAR CELLS

It is one of the most traditional and effective solar cell manufacturing techniques [61]. Based on the production of silicon wafers, there are two types of crystalline solar cells.

- Monocrystalline silicon solar cell
- Multicrystalline silicon solar cell

Monocrystalline silicon solar cells are produced from a single silicon crystal using the Czochralski method. A solar panel is constructed of a number of solar cells arranged in a grid. With an efficiency of around 17–18%, monocrystalline solar cells are more effective than other solar cells and as a result generate more electrical power for a given area than other solar panels. However, the growing of large crystal of pure silicon is energy intensive and difficult process that results into high production cost [61].

Multiple silicon crystals are molded into a single cell to create polycrystalline silicon cells. Manufacturing polycrystalline solar cells is simpler than monocrystalline solar cells. But compared to monocrystalline solar cells, the efficiency of polycrystalline solar cells is between 12 and 14%, which is slightly lower. Around 48% of the world's solar cell manufacturing in 2008 was made up of polycrystalline solar cells, which are widely used [62, 63].

15.6.2 SECOND-GENERATION (2G) SOLAR CELLS

Silicon wafers alone account for about 50% of the cost of production in crystalline solar cells [64]. It can be substituted by a thin semiconductor film that has been placed on a supporting substrate to lower production costs. Crystalline solar cells are more expensive to manufacture than thin-film solar cells. However, thin films' efficiency, which varies from 4% to 10%, hinders widespread use of the technology [64]. There are three varieties of thin-film solar cells:

- Amorphous silicon thin film (a-Si)
- Cadmium telluride (CdTe)
- Copper indium gallium di-selenide (CIGS)

15.6.3 AMORPHOUS SILICON THIN FILM (A-SI) SOLAR CELLS

In contrast to monocrystalline and polycrystalline solar cells, amorphous silicon solar cells are made by depositing a thin layer of silicon onto a metal, glass, or plastic substrate. The production of amorphous silicon cells involves expensive procedures. Amorphous silicon solar cells must have a larger surface area to produce the same amount of power as crystalline solar cells due to their lower efficiency (around 10%). Amorphous solar cells have been mostly used in calculators and other small electrical devices since the early 1980s. The simplicity and easy availability of silicon are advantages of a-Si solar cells. The drawbacks of amorphous silicon TFSCs include poor and variable efficiency as well as light-induced material quality degradation [61, 63, 64].

15.6.4 CADMIUM TELLURIDE (CDTE)

Cadmium telluride (CdTe) solar cells are very popular due to high optical absorption capability and low production costs. Cadmium telluride (CdTe) of 1 μm thickness can absorb 90% of solar spectrum [65]. The manufacturing process is also less complex and requires less material than other solar cell technologies. Cadmium telluride has an efficiency of around 9–11% [63]. However, cadmium is considered as a toxic agent that can be harmful to human and animals. The disposal of cadmium poses a serious environmental issue and as such the application of cadmium telluride poses a serious environmental concern. Two key players, Matsushita and BP Solar, have abandoned technology citing environmental concerns [64].

15.6.5 COPPER INDIUM GALLIUM DI-SELENIDE (CIGS) SOLAR CELLS

Copper, indium, gallium, and selenide make up the four components of the CIGS solar cell, a semiconductor material. Due to their low cost and efficiency of 10–12%, CIGS solar cells are a relatively common thin film technology. The advantages of CIGS solar cell include low costs, better efficiency, and prolonged life [63]. However, the main concern with CIGS technology is the availability of resources. There is a limited availability of indium as total production of solar cell from it would be no more than present capacity of all wind generators [64].

15.6.6 THIRD-GENERATION (3G) SOLAR CELLS

Third-generation solar cells are a more recent technology that is being developed. Various third-generation (3G) solar cell technologies are:

- Nanocrystal solar cell
- Polymer solar cell
- Dye-sensitized solar cell

15.6.7 NANOCRYSTAL SOLAR CELL

A nanocrystal solar cell's substrate is coated with a few quantum dots, which are nanometer-sized crystalline particles. Materials like silicon or TiO_2 are frequently used in quantum dots. A thin film of nanocrystal is obtained through "spin coating" in which a quantum dot is placed on a substrate and then rotated very quickly until solution spread uniformly. In a bulk semiconductor material, one electron–hole pair produced due to the photon excitement. In nanocrystal material, multiple exciton generation property applies where several electron–hole pairs are created due to photon excitation [63]. Thus, nanocrystal solar cells have a higher potential to achieve good efficiency..

15.6.8 POLYMER SOLAR CELL

A photon-absorbing layer is sandwiched between two electrodes placed on a plastic or glass substrate to make up a polymer solar cell. One of the electrodes is transparent allowing photon to penetrate in absorbing layer. Mostly, indium tin oxide is used as transparent electrode and calcium, aluminum, or magnesium are used as another electrode [66]. Due to photon energy, hole and excited electrons are created in the form of exciton. The recombination of holes and electrons usually occurs with the release of absorbed energy. However, in polymer solar cell, the free hole and free electron are transported to different electrodes due to the difference in ionization energy of two electrodes and then both free holes and free electrons recombine through external circuits. Greater flexibility and less weight make polymer solar cells more versatile and easier to utilize in a variety of sizes and shapes. The limitations of polymer solar cells are lower efficiency and faster degradation [67].

15.6.9 DYE-SENSITIZED SOLAR CELL

Working electrode, counter electrode, redox-mediator (electrolyte), and sensitizer (dye) are the four main parts of a dye-sensitized solar cell [63]. Working electrode in a dye-sensitized solar cell sealed to counter electrode covered with a thin coating of electrolyte [68]. Dye-sensitized solar cells are being thought of as a possible replacement for silicon solar cells due to their simple construction, low production costs, and good efficiency of 10–12% even in low light or cloudy conditions. The limitations of dye-sensitised solar cells include temperature-sensitive liquid electrolytes and less efficiency than silicon solar cells [63].

15.7 CONCLUSIONS

This chapter discusses the necessity of a solar PV standalone system and also investigates some of the system's numerous components. Although initially expensive for the user to purchase, a standalone solar PV system pays for itself over time. Solar is a free renewable resource which makes its use more widely in terms of its applications. Areas far away from the grid connection have a great benefit by installing standalone solar panels, which will act as an input source to the running appliances. Therefore, employing solar energy minimizes the need for unconventional resources, which in turn lowers pollution. The demand is seen to be rising daily. It is obvious to make sure that solar energy must be used in a correct way, might be resourceful all the time, but its minimal and optimum usage is must. The correct usage of it leads to more outcomes as compared to any other renewable sources.

We have discussed about various algorithms of MPPT, different topologies of MLI, and DC–DC converters and different systems of connecting solar PV systems. It appears that IC is more effective at high solar irradiation when compared to different algorithms and also, observed that it just needs current- and voltage-determining devices or sensors, by comparing current and the incremental changes that can be estimated. We also conclude that different topologies of DC–DC converter are used because of variable insolation level, the output result of solar module may vary. The output of MPPT is generally given to the PWM for the correct duty ratio as input to DC–DC converters.

The two topology converters are used according to their applications. Buck-boost combination of converter is generally preferred more, operating in continuous conduction mode as to reduce switching stress. Also, as per the output voltage requirements the configuration of circuit changes by adding or reducing certain elements like inductor or capacitor. For buck–boost-type converters, the inductor should be chosen which ensures that saturation current is much higher than inductor peak current.

We also conclude that HBCMLI is more suitable for solar PV applications as compared to other various topologies discussed as it has various advantages such as no flying capacitor or clamping diodes are required, and total harmonic distortion gets reduced drastically when a number of levels of inverter are increased.

KEYWORDS

- **maximum power point tracking**
- **DC–DC converter**
- **Perturb and Observe**
- **incremental conductance**
- **pulse width modulation**

REFERENCES

1. Christopher, W., Ramesh, Dr. R. Comparative study of P&O and InC MPPT algorithms. *Am. J. Eng. Res. (AJER)*, **2013**, *4*, 402–408.
2. Ali, W., Awais, Q., Farooq, H., Jamil, M., Ur Rehman, A., Noman, A. Design consideration of stand alone solar photovoltaic system. In *2018 International Conference on Computing, Electronic and Electrical Engineering (ICE Cube)*.
3. Maity, R., Mathew, M., Hossain, J. Increase in power production of rooftop solar photovoltaic system using tracking. In *2018 International Conference on Power Energy, Environment and Intelligent Control (PEEIC)*.
4. Alghhassab, M. Performance enhancement of stand alone photovoltaic system with household loads. In *2019 2nd International Conference on Computer Application and Information Security (ICCAIS)*, Riyadh, Saudi Arabia, 2019.
5. Lueangamornsiri, T., Thongpull, K., Chalermyanont, K., Wichakool, W. Design and development of a stand alone solar energy harvesting system by MPPT and quick battery charging. In *2016 13th International Conference on Electrical Engineering/Electronics, Computer, Telecommunications and Information Technology (ECTI-CON)*, Thailand.
6. Tudu, B., Mandal, K.K., Chakraborty, N., Mukherjee, I. Stand alone hybrid renewable energy system—an alternative to increase energy demand. In *Proceedings of the 2014 International Conference on Control, Instrumentation, Energy and Communication (CIEC)*.
7. Saha, A., Mishra, S., Progya, P.M. Design and simulation based stand alone solar micro grid system for island areas. In *2019 International Conference on Electrical Engineering Research and Practice (ICEERP)*.
8. Usmani, M.J., Haque, A. Power management of solar PV systems for PEER load. In *2020 IEEE International Conference on Power Electronics, Smart Grid and Renewable Energy (PESGRE 2020)*.
9. Nassereddine, M., Rizk, J., Nagrial, M., Hellany, A. Batter sustainable PV solar house: storage consideration for off Grid. In *2018 3rd International Conference on Electrical and Biomedical Engineering, Clean Energy and Green Computing (EBECEGC)*.
10. Peters, I.M., Watson, S., Sahraei, N., Buonassisi, T. Global design aspects of persistent and autonomous PV powered systems. In *2017 44th Photovoltaic Specialist Conference (PVCS)*.

11. Sharma, A., Koraz, Y., Youssef, M. A novel control methodology for stand alone photovoltaic systems utilizing maximum power point tracking. In *2019 IEEE Canadian Conference on Electrical and Computer Engineering (CCECE)*.
12. Chakraborty, S., Arvind, P., Kumar, D. Integrated solar PV MPPT and V-f control for standalone microgrid. In *2019 International Conference on Electrical, Electronics and Computer Engineering (UPCON)*.
13. Alghassab, M. Performance enhancement of standalone photovoltaic systems with household loads. In *2019 2nd International Conference on Computer Applications & Information Security (ICCAIS)*.
14. Singh, A.K., Gupta, R. Accurate analysis of solar PV module. In *2018 International Conference on Computing, Power and Communication Technologies (GUCON)*.
15. Mohamed, H.A., Khattab, H.A., Mobarka, A., Morsy, G.A. Design, control and performance analysis of DC-DC boost converter for standalone PV system. In *2016 18th International East Power Systems Conference (MEPCON)*.
16. Jiann-Fuh, H.L., Wu, T.-H., Huang, Y.-C., LED driving circuit with standalone photovoltaic power. In *3rd International Future Energy Electronics Confernce and ECCE Asia (IFEEC 2017-ECCE Asia)*.
17. Azad, M.L., Das, S., Sadhu, P.K., Satpati, B., Gupta, A., Arvind, P. P&O algorithm based MPPT technique for solar PV system under different weather conditions. In *2017 International Conference on Circuit, Power and Computing Technologies (ICCPCT)*.
18. Sher, H.A. A new sensorless hybrid MPPT algorithm based on fractional short-circuit current measurement and P&O MPPT. In *IEEE and Marcello Chiaberge*.
19. Divyasharon, R., Banu, R., Devaraj, D. Artificial neural network based MPPT with CUK converter topology for PV systems under varying climatic conditions. In *2019 IEEE International Conference on Intelligent Techniques in Control, Optimization and Signal Processing (INCOS)*.
20. Wang, H., Li, B. The cooperated MPPT control of standalone PV power generation system. In *Proceedings of the 8th World Congress on Intelligent Control and Automation,* Jinan, China,, July 6–9, 2010.
21. Vyas, A.K., Dhiman, H.S. Predication of negative dispersion for photonic crystal fiber using extreme learning machine. *J. Opt. Commun.*, **2021**, 000010151520210124. https://doi.org/10.1515/joc-2021-0124.
22. Dixit, A., Tiwari, S., Vyas, A.K., Kumar, R., Pandey, A. Optimization of hexagonal boron-doped silicate photonic crystal fiber to obtain near zero flattened dispersion for nonlinear waves by finite difference method quantum and optical electronics. *Opt. Quant. Electron.*, **2022**, *54*, 565.
23. Abdourraziq, M.A., Maaroufi, M., Ouassaid, M. A new variable step size INC MPPT method for PV systems. In *2014 International Conference on Multimedia Computing and Systems (ICMCS)*.
24. Jain, K., Gupta, M., Bohre, A.K. Implementation and comparative analysis of P&O and INC MPPT method for PV system. In *2018 8th IEEE India International Conference on Power Electronics (IICPE)*.
25. Ryu, D., Kim, Y.J., Kim, H., Optimum MPPT control period for actual insolation condition. In *2018 IEEE International Telecommunications Energy Conference (INTELEC)*.
26. Ding-hao. A fast RBFN based MPPT method for application of triple junction solar cell. In *2017 9th International Conference on Human Machine System*.

27. Chao, R.-M., Jhang, J.-C., Wang, K., Hus, S.-C. Hardware implementation of a distributed PV system based on central operation of MPPT algorithm. In *The 2017 4th International Conference on Systems and Informatics (ICSAI 2017)*.
28. Morales, M., Morales, R. Digital simulation of a predictive current control for PV system based on the MPPT strategy. In *2016 13th International Conference on Power Electronics*.
29. Andaloussi, Z.J., Raihani, A., Elmagri, A. Toward an approach to improve MPPT efficiency for PV System. In *2017 International Conference on Wireless Technologies, Embedded and Intelligent Systems (WITS)*.
30. Harrag, A., Sabir, Daili, Y. Innovative single sensor neural network PV MPPT. In *2019 6th International Conference on Control, Decision and Information Technologies (CoDIT'19)|,* April 23–26, 2019, Paris, France.
31. Latif, T., Hussain, S.R. Design of a charge controller based on SEPIC and Buck topology using modified incremental conductance MPPT. In *8th International Conference on Electrical and Computer Engineering,* Dhaka, Bangladesh, 20–22 December, 2014.
32. Dong, Y., Ding, J., Huang, J., Xu, L., Dong, W. *Investigation of PV inverter MPPT efficiency test platform*. *International Conference on Renewable Power Generation (RPG 2015)*, China, 2015.
33. Haji, D. Fuzzy and P&O Based MPPT controllers under different conditions. In *7th International Conference on Renewable Energy and Application*.
34. Haji, D., Genc, N. Fuzzy and P and O based MPPT controllers under different conditions. In *7th International Conference on Renewable Energy Research and Applications*.
35. Vyas, A.K., Hiran, K.K., Dhiman, H., Modelling of symmetrical quadrature optical ring resonator with four different topologies and performance analysis using machine learning approach. *J. Opt. Commun.*, **2023**, *44*, s327–s337. https://doi.org/10.1515/joc-2020-0270
36. Singh, A. MATLAB /SIMULINK simulation of PV system based on MPPT in variable irradiance with EV battery as load.
37. Gules, R., De Pellegrin Pacheo, J., Hey, H.L., Imhoff, J. A maximum power point tracking system with parallel connection for PV standalone applications. In *IEEE Transactions on Industrial Electronics*, **2008**, *5*(7).
38. Prakash, S., Kalpana, R., Singh, B. Solar photovoltaic array fed Push-pull buck DC-DC converter for telecom load. In *2017 14th IEEE India Council International Conference (INDICON)*.
39. Nakajima, A., Masukawa, S. Study of boost type DC-DC converter for single solar cell. In *IECON 2018—44th Annual Conference of the IEEE Industrial Electronics Society*.
40. Ali, S., Babak, A., Mohsen, H. A non-isolated buck-boost DC-DC converter with continous input current for photovoltaic applications. *IEEE J. Emerg. Sel. Top. Power Electron*. **2020**, *9*(1), 804–811.
41. Babaa, S., Armstrong, M., Pickert, V. High efficiency standalone photovoltaic system using adaptive switching of an interleaved boost converter. In *6th IET International Conference on Power Electronics, Machines and Drives*.
42. Saravanan, S., Ramesh Babu, N. Design and development of single switch high step -Up DC-DC converter. *IEEE J. Emerg. Sel. Top. Power Electron.*, **2018**, *6*(2).
43. Das, M., Agarwal, V. Novel high-performance standalone solar PV system with high gain, high efficiency DC-DC converter power stages. *IEEE Trans. Ind. Appl.*, **2015**, *51*(6).
44. Li, R., Shi, F. Control and optimization of residential photovoltaic power generation system with high efficiency isolated bidirectional DC-DC converter. **2019**, *7*.

45. Bhagiya, R.D., Patel, R.M. PWM based double loop PI control of a bidirectional DC-DC converter in a standalone PV/Battery DC power system. In *2019 IEEE 16th India Council International Conference (INDICON)*.
46. Matwankar, C.S., Alam, A. Solar powered closed-loop current controlled DC-DC Buck converter for battery charging application. In *2019 International Conference on Vision Towards Emerging Trends in Communication and Networking*.
47. Anand, I., Senithilkumar, S., Biswas, D., Kaliamoorthy, M. Dynamic power management system employing single stage power converter for standalone solar PV applications. In *2018 IEEE Transactions on Power Electronics*.
48. Bhattacharya, S., Samanta, S. 2020 In *IEEE International Conference on Power Electronics, Smart Grid and Renewable Energy (PESGRE2020)*.
49. Liao, Z., Ruan, X. Control strategy of Bi-directional DC-DC converter for a novel standalone photovoltaic power system. *IEEE Vehicle Power and Propulsion Conference (VPPC)*, Harbin, China, September 3–5, 2008.
50. Mitra, L., Kumar Rout, U. Double input DC-DC converter with PV and DC source for standalone applications. In *2016 International Conference on Microelectronics, Computing and Communications (MicroCom)*.
51. Harsha, C.M., Angadi, J. High performance DC-DC converter for low voltage standalone solar PV systems. In *2017 International Conference on recent advances in Electronics and Communication Technology*.
52. Patil, S.N, Prasad, Dr. R.C. Design and development of MPPT algorithm for high efficient DC-DC converter for solar energy system connected to grid. In *2015 International Conference on Energy System and Applications*.
53. Shah, B., Kumar, G.V.E.S. A comparative study of different MPPT techniques using different DC-DC converter in a standalone PV system. In *2016 IEEE Region 10 Conference Paper*.
54. Kale, A.S., Tamhane, A.V., Kalage, A.A., Comparative study of SPWM And SVPWM cascaded h-bridge multilevel inverter. In *2017 International Conference on Intelligent Computing and Control (I2C2)*, Coimbatore, India, 2017.
55. Yao, W., Hu, H., Lu, Z., Comparisons of space-vector modulation and carrier-based modulation of multilevel inverter. In *IEEE Trans. Power Electron.*, *23*(1), 45–51.
56. Rodriguez, J., Lai, J.-S., Peng, F.Z., Multilevel inverters: a survey of topologies, controls, and applications. In *IEEE Trans Indus Electron.*, *49*(4), 724–738.
57. Awad, A.A., Abdalla, O.H., Norallah, H., Jibril, M.I., Series parallel cascaded H-bridge inverter based on a simple staircase modulation. In *2019 International Conference on Computer, Control, Electrical, and Electronics Engineering (ICCCEEE)*, Khartoum, Sudan, 2019.
58. Sankar, D., Babu, C.A., Cascaded H bridge multilevel inverter topologies for PV application: a comparison. In *2016 International Conference on Circuit, Power and Computing Technologies (ICCPCT)*, Nagercoil, Tamil Nadu, India, 2016.
59. Maurya, S., Mishra, D., Singh, K., Mishra, A.K., Pandey, Y. An efficient technique to reduce total harmonics distortion in cascaded H-bridge multilevel inverter. In *2019 IEEE International Conference on Electrical, Computer and Communication Technologies (ICECCT)*, Coimbatore, India, 2019.
60. Vyas, A.K. Elliptical air holes based photonic crystal fiber for narrow band gap and peak power at 1.55 micrometre wavelength. *Optik*, **2019**, *184*, 28–34.

61. Ranabhat, K., Patrikeev, L., Antal'evna-Revina, A., Andrianov, K., Lapshinsky, V., Sofronova, E. An introduction to solar cell technology. *J. Appl. Eng. Sci.*, **2016**, *14*(4), 481–491.
62. Imamzai, M., Aghaei, M., Hanum Md Thayoob, Y., Forouzanfar, M. A review on comparison between traditional silicon solar cells and thin-film CdTe solar cells. In *Proceedings of National Graduate Conference*, 2012, pp 1–5.
63. Saga, T. Advances in crystalline silicon solar cell technology for industrial mass production. *NPG Asia Mater.*, **2010**, *2*, 96–102
64. Sharma, S., Kumar Jain, K., Sharma, A. Solar cells: in research and applications—a review. *Mater. Sci. Appl.*, **2015**, *6*(12), 1145.
65. Green, M.A. Thin-film solar cells: review of materials, technologies and commercial status. *J. Mater. Sci. Mater. Electron*, **2007**, *18*, 15–19.
66. Asim, N., Sopian, K., Ahmadi, S., Saeedfar, K., Alghoul, M.A., Saadatian, O., Zaidi, S.H. A review on the role of materials science in solar cells. *Renew. Sustain. Energy Rev.*, **2012**, *16*(8), 5834–5847.
67. Spanggaard, H., Krebs, F.C. A brief history of the development of organic and polymeric photovoltaics. *Sol. Energy Mater. Sol. Cells*, **2004**, *83*(2–3), 125–146.
68. Sharma, K., Sharma, V., Sharma, S.S. Dye-sensitized solar cells: fundamentals and current status. *Nanoscale Res. Lett.*, **2018**, *13*(1), 1–46.

CHAPTER 16

4D PRINTING: FUNDAMENTALS, MATERIALS, APPLICATIONS AND CHALLENGES

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ABSTRACT

A device or object that can change from a one-dimensional (1D) strand into a preprogrammed three-dimensional (3D) shape, from a two-dimensional (2D) surface into a preprogrammed 3D shape, or that can morph between multiple dimensions is said to be printed in four dimensions using a single substance or a combination of materials. Electrochemically, by programming varied sensitivity to, for example, swelling into distinct regions of the planned shape, and by applying various stimuli, such as heating, light, or swelling in a liquid, these transformations are made possible. These methods promise new ways to embed programmability and straightforward decision-making into nonelectronic-based materials while providing adaptability and dynamic responsiveness for buildings and systems of all sizes. The development of four-dimensional (4D) printing as a standard production technology represents a revolutionary leap in manufacturing, integrating time as a critical design dimension. In this chapter, we cover the fundamentals and regulations regulating 4D printing, the materials used in 4D printing, as well as some of the applications, including soft robotics, and the difficulties that must be overcome before 4D printing can become a commonplace manufacturing process.

16.1 INTRODUCTION

The development and advancement of three-dimensional (3D) printing technology is where the history of four-dimensional (4D) printing begins. Therefore, it is crucial to understand the history of 3D printing (3DP), which eventually gave way to the development of 4D printing. The reader will grasp the concept of 4D printing and its evolution better if they have a basic understanding of 3DP, including its history, printing processes, etc. A method of producing basic or complicated structures layer by layer using computer-aided design is known as 3DP. When Chuck Hull (of 3D Systems Corp.) submitted a patent for the stereolithographic technique, the field of 3DP experienced a surge. Later, at MIT (Massachusetts Institute of Process), the adhesive jetting process using a powder bed was linked to the phrase 3DP. Another name for industrial-scale 3DP is additive manufacturing (AM), often known as rapid prototyping. Currently, the media and consumer communities employ 3DP technology in a variety of printing processes, including stereolithography (SLA) [1], selective laser sintering (SLS), fused deposition modeling (FDM), and jet 3DP. Due to its ability to produce goods with high speed, high accuracy, and low cost, 3DP has sparked a lot of interest among academic institutions and major corporations. The multidisciplinary nature of 3DP necessitates the collaboration of numerous scientific and technological disciplines, including material science [2], mechanical engineering, data processing, etc. Recent advances in 3DP have made it possible for researchers to build sophisticated structures that were previously unattainable using older, more conventional techniques are all examples of successful research projects.

The two most popular methods for 3DP are SLA and FDM. FDM employs a heated nozzle to deposit molten material on a bed layer by layer while SLA prints with a laser. In addition to these, 3DP processes such as powder bed fusion, material extrusion, binder jetting, material jetting, sheet lamination, vat photopolymerization, and directed energy deposition (DED) are frequently utilized. Since 3DP can produce complicated structures, there has been a significant advancement in research and development in this field. Due to its lengthy cycle time, it is currently not ready for widespread use [3].

The barrier in 3DP technologies is increased by the shortage of printing materials with excellent performance. Additionally, the creation of mostly static structures using one or more materials is the core emphasis of 3DP. As a result, 3DP cannot satisfy the requirements in applications where a dynamic function is required. Self-folding packaging, adaptable wind turbines, and soft grippers for surgical uses are a few examples of these dynamic features. Shape memory polymers (SMP) significantly enhance the mechanical and structural qualities of wind turbine blades, according to research by Momeni et al. These SMPs-based blades were created in a single print cycle, which adds a fourth dimension–time-to 3DP. 4D printing, which was made possible by the addition of a fourth dimension to 3DP, is a relatively recent printing technology. This essay is broken into several sections, and we will start by talking about the fundamentals, materials, and methods of 4D printing. Then, in the final section of the essay, we will concentrate on its application and potential future application.

16.2 4D PRINTING

Skylar Tibbits demonstrated how changes take place over time in a static produced item (via 3DP) at the Technology, Entertainment, Design conference held at MIT in 2012. A simple 3D structure has been shown to evolve over time into a more complicated structure. As a result, a new era of printing emerged that added a 4D to 3DP—time—and was dubbed 4D printing technology. Time is the fourth dimension, thus we can simply state that 4D printing equals 3DP plus an additional dimension of time. Or we could say that when 3D printed materials evolve through time, 4D printed materials emerge. Following Tibbits' speech, 4D printing began to gain traction among scientists and engineers working in a variety of fields. A year after the TED lecture, the first 4D printing research article was released. In this study, the idea of printed active composites (PACs) was employed to use the shape memory effect (SME) to turn a printed sheet into a complex structure. Since then, 4D printing research has proliferated globally at an exponential rate. One of the fundamental features of 4D printing is that it can change shape over time with the aid of a computer command that has been preprogrammed. For 4D printing, many definitions have been developed. The first was that 4D printing was really 3DP that had been given more time. The 4D printing definition, however, states that it is "the evolution in the shape, property, and functionality of a 3D printed structure with time when it is exposed to heat, light, water, pH, etc." Another definition of 4D printing that sums it up wonderfully is "4D printing is the fabrication of items that change shape when taken out of a 3D printer." Due to the chemical interaction of the materials utilized, these things self-assemble when exposed to water, heat, and air, among other factors. Combining a 3D printer, intelligent material, and a carefully planned design is known as 4D printing.

In 4D printing, different metamaterial structures are formed as a result of environmental changes. The majority of 4D printing research now being conducted focuses on the capability of changing shape, including elongation, materials created via 4D printing can be bent, corrugated, and twisted. The 4D printed materials are ideal for creating toys because of these capabilities, microtubes, lockers, lifters, robots, and lockers.

16.2.1 FACTORS RESPONSIBLE FOR 4D PRINTING

The five criteria are mostly what 4D printing depends on, and while using 4D printing, all five factors must be taken into consideration. These five elements are the AM technique, the printing medium, the stimuli, the interaction mechanism, and modeling.

The printing method employed in the AM is the first component. Without the need for an intermediary tool, the AM technique permits the creation of printing material from digital information provided by the computer. Numerous AM techniques exist, including SLA, SLS [4], FDM, jet 3DP, selective laser melting (SLM), direct ink writing (DIW), electron beam melting [5], etc. Almost all of these techniques can print a 4D material so long as the printing medium is appropriate for the printer.

The second consideration is the printing medium, which needs to respond to stimuli while being sandwiched layer by layer. These materials are also referred to as smart materials (SMs) or programmable materials [6]. The nature of these SMs decides the stimuli that will be employed, and the way that these materials react to the stimuli determines their capacity for self-transformation.

The stimuli used in 4D printing constitute the third aspect or factor. Physical, chemical, and biological stimuli are all possible. Light, moisture, magnetic and electric energy, temperature, UV light, and other physical stimuli are among them. Chemicals, pH, oxidant, and reductant use are examples of chemical stimuli. The biological stimuli also include glucose and enzymes. When a stimulus is introduced, the structure experiences physical or chemical changes, such as relaxation of stress, molecular motion, and phase changes, which cause the structure to deform.

The interaction mechanism and mathematical modeling make up the fourth and fifth factors [7], respectively. Not all materials are capable of undergoing the necessary transformation when a stimulus is applied to SM. We must offer an interaction method that will plan the sequence of form change, such as mechanical loading or physical manipulation. The mathematical modeling is necessary to determine the duration for which the stimulus will act upon the SM after supplying the interaction mechanism. Given the driving forces behind 4D printing, it may be summarized as follows: “The stimulus is applied on the smart material using a suitable interaction mechanism and mathematical modeling during an AM process, which results in a 4D printed structure.”

16.2.2 LAWS OF 4D PRINTING

Three rules were developed by F. Momeni and J. Ni to describe the shape-changing behavior of all 4D printed structures. These principles offer a clearer picture of the physics underlying the ability of 4D-printed things to change shape. The following laws are listed:

16.2.2.1 FIRST LAW

According to the first law, “all the shape-changing behaviors of multimaterial 4D structures, such as coiling, curling, twisting, bending, etc. are due to the relative expansion between active and passive materials.”

16.2.2.2 SECOND LAW

According to the second law, “all multimaterial 4D structures have the ability to change shape due to four physical factors: mass diffusion, thermal expansion, molecular transformation, and organic growth.” All of these elements contribute to the relative expansion between active and passive materials, which causes shape change in response to a stimulus.

A change in the structure’s mass results from the absorption or adsorption of stimuli (such as water or ions). This movement of stuff eventually causes the material to expand relatively, changing the substance’s shape. When electrical, thermal, chemical, or other stimuli are utilized, the mass change can also happen. Because the average distance between atoms and molecules changes with temperature and consequently with relative expansion, thermal expansion can result in structural deformations. In fact all of these stimuli can alter the structure’s temperature, thermal expansion can also happen when electrical, light, and UV stimuli are employed. Relative expansion can happen in the structures as a result of molecular transformation when the mass and temperature of the structure are constant. In these situations, a variety of fields, including electric, magnetic, optical, and mechanical ones, can trigger molecular change. For instance, when an electric or magnetic field is applied, the material's dipoles will align themselves in accordance with the direction of the field, which will cause molecules to change. Similar results are obtained when mechanical strain is applied to polymers, which causes the chains to align in a specific orientation, and when UV light is applied to photosensitive materials, which causes trans-to-cis conversion. Organic growth is the gradual increase in length and mass of a living organism [8]. A relative expansion of active and passive materials will happen as weight and length grow, leading to behavior that changes shape. Electrical impulses can be used to primarily promote organic growth in biological things. In addition, we can employ other things like heat, water, pH, mechanical force, etc. The shape-changing behavior of cells, tissues, scaffolds, stents, organs, etc. created through 4D bioprinting is referred to as "organic growth."

16.2.2.3 THIRD LAW

According to the third law of 4D printing, "nearly all multimaterial 4D printed structures exhibit time-dependent shape-morphing behavior that is governed by two 'types' of time constants." Depending on the stimuli and material used for 4D printing, these constants may be equal, big, or disappear in relation to one another. Additionally, a mathematical bi-exponential formula for the fourth dimension was developed, which can be applied in the future to the modeling of 4D structures using hardware and software.

16.2.3 TYPE OF MATERIALS USED IN 4D PRINTING

Recent advancements in 3DP have made it possible to arrange materials more precisely and flexibly, which has greatly aided 4D printing. In addition to using materials that may change shape, 4D printing also uses materials that can change color when exposed to UV and visible light. Based on how they react to stimuli, the many types of SMs utilized in 4D printing will be covered in this section.

16.2.3.1 MATERIALS RESPONSIVE TOWARD MOISTURE: HYDROGELS

Due to their many potential uses, materials that are sensitive to moisture or water have drawn a lot of attention. These materials are also known as hydrogels because of their exceptional capacity to react to moisture or water. They are actually a group of crosslinked 3D networks of polymer chains that may expand to 200% of their original volume when in contact with moisture. As many structures have been created utilizing hydrogels capable of folding, bending, stretching, and geometric expansion, hydrogels also have a high printing capability. When utilized with DIW, they are extremely biocompatible and simple to print.

The hydrophobic films made from cellulose stearoyl esters by Zhang et al. responded more quickly and precisely than the earlier ones [9]. Typically, hydrogels are submerged in water and allowed to absorb the water until they reach their saturation point. However, this technique has the drawback of restricting hydrogels' ability to alter their behavior at intermediate levels. We can alter the aqueous medium's temperature to get around this. Breger et al. made a demonstration of this when they used hydrogels made of (poly-*N*-isopropylacrylamide-*co*-acrylicacid) pNIPAM-AAc to create the micro-gripper joint. Reverse actuation was accomplished when the temperature of the water in which the gripper was submerged was altered. Alginate/pNIPAM ICE gel inks were also used by G.M. Spinks et al. to print 4D materials. Tibbits et al. also showed how hinge designs can be used to prevent over-swelling. They created a self-folding structure using PolyJet printers that would cease folding at specific preprogrammed angles to prevent excessive swelling.

16.2.3.2 MATERIALS RESPONSIVE TOWARD TEMPERATURE: THERMO-RESPONSIVE

These are the intelligent materials that react to stimuli involving heat or temperature. Two mechanisms—the shape change effect (SCE) or the SME—are primarily responsible for these materials' form alterations in response to thermal stimuli. SME is the use of external stimuli to restore the original shape of a distorted (plastic) material. The SMMs may display SCE in addition to SME depending on the environmental factors. Due to their ease of printing, SMPs are the form of SMM that researchers utilize the most frequently. The SMPs can be distorted with the proper stimulation and then return to their original shape.

The typical glass transition temperature (T_g) of SMPs is greater than the temperature range in which they are typically used. They are programmed above T_g and under specified thermal and mechanical circumstances, and when cooled, they have a transient shape that is not subject to external loads.

Moreover they maintain their original shape when the temperature is once more raised above T_g [10]. This is because the internal energy of polymer chains below T_g is low and they are unable to move freely, causing the material to become glassy and hard. The researchers have altered SMPs in order to utilize their unique properties for printing purposes, such as thermoset and SMPs for thermadaption. In addition to these, SMHs are intelligent materials created by fusing hydrogels, SMPs, and SMAs. These are capable of responding to pressure, temperature, and many inputs simultaneously.

When it comes to SCE materials, the deformation varies between extreme states or is proportionate to the applied stimulus. Such pronounced alterations in the form necessitate a sudden change in temperature.

16.2.3.3 MATERIALS RESPONSIVE TOWARD THE LIGHT: PHOTO-RESPONSIVE

Additionally, light serves as a subliminal cue for the deformation of intelligent materials. When a portion of a SM—also known as a photoresponsive material—is exposed to light, the area absorbs the light, which eventually causes the heating phenomenon in the material. Additionally, as was previously said, heat works as a stimulant for the deformation of SMs, causing the photoresponsive material to alter shape. Because light does not bring about a change directly like heat and moisture do, it functions as an indirect stimulus. Liu et al. presented a sequential self-folding construction where the light is absorbed by the joints and they heat up causing the shape change. The type of lighting used and the color of the joints both affect how quickly heat is absorbed by the joints. Kuksenok et al. employed light in a different method in a different study to cause deformation in the photoresponsive material. They injected a chromophore—a substance that is photosensitive—into a few chosen regions of a polymer block (gel), causing just those regions to deform when light is shone upon the structure [11].

16.2.3.4 MATERIALS RESPONSIVE TOWARD THE ELECTRIC ENERGY: ELECTRO-RESPONSIVE

Electricity is a similar indirect stimulation to light in that it has been demonstrated to have a heating impact on the materials it passes through. The so-called electro-responsive materials are those that deform as a result of their responsive behavior to the electric current. A silicon elastomer and ethanol mixture was used by Miriyev et al. to create an artificial muscle. When current is applied to a muscle, the ethanol evaporates, increasing the volume of the muscle and ultimately causing deformation or expansion of the muscle. Electricity can influence the absorption or desorption of water in polypyrrole (PPy), and Okuzaki et al. used this idea to create microrobots (origami) out of PPy.

16.2.3.5 MATERIALS RESPONSIVE TOWARD MAGNETIC ENERGY: MAGNETO-RESPONSIVE

Another indirect stimulus that might cause deformation in SMs is the magnetic field or the magnetic energy. Additionally, materials that deform in reaction to magnetic energy are referred to as magneto-responsive materials since they are utilized to print 4D structures. Breger et al. used magnetic nanoparticles in a microgripper (printed from hydrogel) to accomplish a remote-control mode. The printed structure started to exhibit responsiveness that can be controlled by a remote when a magnetic field was applied to it. With the exception of the need that the print size be small and light, 4D printed structures made of magneto-responsive materials offer tremendous promise for use in the field of metal and polymer printing.

16.2.3.6 PIEZOELECTRIC MATERIALS

When subjected to mechanical stress, piezoelectric materials have the ability to generate a charge. Piezoelectricity is the process of creating electric charges as a result of a mechanical force. Piezoelectric materials are also suitable for 4D printing since they may distort when subjected to mechanical forces. The phenomenon is straightforward: when stress is applied, charges are generated, and these charges eventually cause the structure to alter (because charges can result in deformation).

16.2.3.7 MATERIALS RESPONSIVE TOWARD PH

These are intelligent materials that can adapt to pH levels and change their structure and volume accordingly. They are suitable for 4D printing technology because of the shape distortion that occurs in response to varying pH values. Since polyelectrolytes feature an ionizable side group [12], they can accept or give protons when the pH value changes, making them pH-responsive polymers that have been employed in 4D printing. Electrostatic repulsion causes the polymer chain to stretch when a proton is released, deforming the structure. When a proton is accepted, the structure returns to its original shape. Polyelectrolytes have polyanions or polyacids (carboxyl or sulfonic groups) as the functional group and polycations or polybases (such as ammonium salt) as the structural component. At higher pH levels, the side chains release the proton (stretch), while at lower pH levels, they take the proton (neutralize). While the functional group accepts the proton at higher pH levels and releases it at lower pH levels [13]. Drug delivery is just a few areas where pH-responsive materials have found use.

Following its introduction, 4D printing has been predicted to have a wide range of applications in numerous scientific and technological domains. This technology has significantly decreased the amount of space needed for storing in printed structures and has made it possible to modify different elements of printed devices and structures. Simply put, 4D printing has made printing dynamic, giving researchers the freedom to select various techniques and materials according on their needs. In contrast, 3DP was static and used the same material for a variety of purposes. The researchers have concentrated their efforts on the 4D-printed structures because of their dynamic properties. When we examine these 4D-printed structures closely, we discover that their capacity for self-assembly and self-repair increases their potential for a range of uses. They can be utilized, for instance, to create surgical tools that can pierce the body and then self-assemble where they are needed. The three characteristics of the 4D-printed structures—self-assembly, self-adaptability, and self-repair—have increased their viability in various applications.

16.2.3.8 SELF-ASSEMBLY

This is the capacity of a SM to join together to build distinct 3D-printed structures before evolving into a challenging 4D structure. When employed in severe environmental conditions, such as space, 4D-printed materials can be quite useful. Transporting such 4D-printed goods to space stations is an option. Additionally, this capability can be exploited to build satellites and antennae since the components can self-assemble in space. This will speed up and improve the quality of the construction. However, it should be highlighted that not every application will benefit from the 4D-printed materials' ability to self-assemble. When such an operation is necessary, this characteristic will prove useful.

16.2.3.9 SELF-ADAPTABILITY

The structures that are 4D printed are capable of adapting to their surroundings and conditions and making the appropriate structural modifications. For instance, a certain 4D printed material may assemble quickly in some circumstances while taking longer to construct in others. This could be referred to as the material's self-capability. Additionally, as was previously mentioned, some materials undergo shape and structure changes as they are heated and cooled. This could be interpreted as their ability to change themselves to fit the circumstances. This property of the 4D-printed materials can be highly useful in building self-adaptive medical devices and tissues. Moreover, electromechanical systems can make use of this characteristic.

16.2.3.10 SELF-REPAIR

The ability of 4D printed materials to self-correct mistakes and flaws makes them particularly valuable in a variety of applications. Self-repair is the common term for this characteristic. For instance, many self-repairing 4D printed materials might be highly useful in applications where we need self-healing (pipes), recycling, etc. The production of self-healing inks (hydrogels) has already begun, but there are still more applications for these materials' inherent ability to fix themselves. It is unnecessary to reiterate the requirement to identify the uses for self-repairing in 4D printed materials in order to achieve better outcomes.

16.3 4D PRINTING TECHNIQUES

As far as we are aware, 4D printing is an improvement over 3DP. The AM printing methods are the ones utilized in 4D printing. We will briefly go through the various printing processes utilized in 4D printing in this part. The printing method is called FDM.

Using the FDM printing method, the substance to be printed is extruded through a nozzle and hardened on a substrate. A motor that supports the nozzle enables it to move in the X and Y axes. The nozzle is raised in the Z-axis after a 2D layer [14–23] is produced on a substrate to print a layer on top of the previously printed layer. In this manner, layers are added one at a time until a final 3D or 4D printed structure is achieved. Due to its low maintenance and consumables costs, FDM is commonly utilized for both 3D and 4D printing. Regular changes have been made to the FDM process to make it compatible with printing new materials. For the 3DP of composites like continuous fiber-reinforced thermoplastic composites (CFRTC), Tian et al. research focused on the use of FDM printing for SME materials. They ran models and manufactured structures with SME capabilities using FDM printing. FDM is commonly used in 4D printing, and research is being done to improve it and make it compatible with new materials.

Another printing method utilized in 4D printing technology is SLA. This method makes use of a photopolymer, a substance that responds to light and solidifies. The material can be solidified using a variety of radiations, including UV light, visible light, X-rays, electron beams, etc. On a larger scale, however, only UV and visible lights are employed. SLA has been used effectively to build challenging and complicated structures. Additionally, materials that work with the SLA printing method have been created.

SLS printing with a Stratasys Connex printer and UV light was used for the first novel 4D printing project. Additionally, depending on the situation, the laser's intensity and beam speed can be changed. SMAs are typically printed using SLM.

Another sort of AM technology is DED. Although it may be used with polymers and ceramics, printing metal pieces is its primary use. Other methods include DIW printing and projection micro stereolithography, which are mostly used for 4D printing's biomedical applications. A large variety of materials can be printed using the DIW method, which is comparable to FDM printing. Inks for DIW can be made from thermoplastics, hydrogels, sol–gel oxides, polyelectrolytes, etc.

16.4 APPLICATIONS OF 4D PRINTING

This section will go through some of the scientific fields where using 4D material has been beneficial so that the reader will be introduced to these many sectors and perhaps achieve some exceptional outcomes in the future. The 4D printing technology is still in its early phases of development, but it has already attracted a lot of attention from numerous research and technological disciplines. A program to create 4D printed materials that can be useful in the sphere of defense and protection has already been launched by the US Army at three separate colleges. As an illustration, 4D-printed coatings for defense vehicles can adjust to various environmental conditions and alter their shape. The impact of 4D printed materials on people's daily lives is astounding. In consideration of user requirements, printed objects can adjust to shifting environmental conditions (humidity, temperature, pressure, wetness, etc.). Additionally, since 4D printed products take up less volume, less space and labor will be needed for their shipping and assembly. Because of their ability to function independently and repair themselves, the products can be employed to satisfy new demands after being used. The potential for their use in space-related programs is enormous. It is possible to 4D print the solar cells and antenna used in satellites and spacecraft. They can self-assemble in place, decreasing labor requirements, and they can also adjust to the changing conditions of the environment. A potential application for 4D printed structures is in the medical sciences. Through a small incision, 4D-printed stents can be inserted into the body, and once they are in the correct location, they can be altered by external stimuli to provide the desired effects. Additionally, a nano 4D-printed gadget can be inserted into the body; it will self-assemble once it reaches the necessary spot and perform the intended operation. In the area of robotics and actuators, where they can be employed to develop technology, printing has also experienced tremendous success. In robotics, 4D-printed [24–28] structures can take the place of costly components like motors, sensors, and difficult-to-assemble materials. Additionally, the use of these materials will result in smaller robots. Self-healing hydrogels, self-healing pipes, and fixing building flaws are just a few of the potential uses for 4D printed materials that are anticipated in the future. The fields of sensors and printed artificial organs can both benefit from the use of these printed materials.

16.4.1 MEDICAL APPLICATIONS

The use of the material transfer method known as “bioprinting” to create biological materials such as cells, tissues, chemicals, etc. in order to carry out biological tasks. The rise in organ transplants led to the development of the discipline of bioprinting. The lack of available organs for transplant and the limits of conventional tissue engineering eventually led to the creation of a new subset of tissue engineering known as 3D or 4D bioprinting. When compared to conventional tissue engineering, bioprinting has a number of advantages, including the ability to create tissues with a high density and construct huge tissue-engineered objects. As technology developed over time, 3D bioprinting became 4D bioprinting. The process of printing biocompatible materials in three dimensions that can change over time is known as 4D bioprinting. 4D bioprinting involves the maturation of a 3D printed structure utilizing a biomaterial (that can alter shape). This is one of the sectors that is expanding as a result of the use of 4D printing, where we can create models of different organs to research their behavior and makeup in order to develop better treatments for diseases that affect those organs. To track the physical changes in cells and tissues, 4D-printed nanobiomedical devices, such as biosensors, bioactuators, and biorobots, can be very useful.

The biorobots may carry out surgery as well as distribute therapeutics and medications. By taking advantage of their self-deformation, 4D printing can be particularly effective in addressing abnormalities in the field of orthopedics. The generated orthopedic models can also alter their characteristics in response to applied stimuli. The orthopedic components made using 4D printing are more flexible, may be a precise reproduction of the patient's portion, and can be used successfully in difficult procedures. When medication is needed at a particular spot, 4D-printed devices can be employed to administer the treatment. When the surroundings at the chosen site are suitable for serving as stimuli, they can contain the medication and release it. "Theragrippers" were created by Malachowski et al. to deliver drugs to specific targets in the gastrointestinal system. As a result, 4D printing has enormous potential in the field of medicine, where it has the potential to enhance clinical results, reduce surgical difficulties, fabricate scaffolds and stents for dental applications, target drug delivery, and offer accurate information about human anatomy.

16.4.2 APPLICATION IN SOFT ROBOTICS

Hard materials like metals, tough polymers, and ceramics are frequently employed to create robots in conventional robotics. To get over these restrictions, the discipline of soft robotics was created, which can create robots that are flexible like humans, can change their stiffness, and can adapt to their surroundings. The inability to print one fully assembled DEA at a time is another drawback of this approach. However, work can be done in this area in the future such that the structures would not need prestraining and will be helpful in soft robotics. Soft robotics can also benefit from the usage of soft actuators (SA).

A composite material that can be utilized as SA was created by Miriyev et al. However, this is still in its early phases of development, and no promising research in this area has yet to be published. As a result, 4D printing has enormous promise for use in soft robotics, but more materials of this type will need to be created in the future to enable improved actuation and control.

Another issue that needs to be resolved in the future is the durability and actuation performance of 4D-printed robotics.

16.4.3 APPLICATION AS SELF-EVOLVING STRUCTURES

Self-evolving structures that can regain their previous shape upon contact with water can be created using 4D printing. These were initially created by Raviv et al. utilizing various multimaterials, and the study team also gave them names. A hydrophilic polymer was used to print the structure over a plastic substrate; the polymer would expand in volume when exposed to water. The group created numerous intricate structures that displayed deformations including folding and stretching. The structures' mechanical degeneration was brought on by the constant wetting and drying of the structures. However, these issues can soon be resolved by investigating novel multimaterials with self-evolving properties. Additionally, other causes, like as temperature and UV exposure, can be investigated for such materials in addition to moisture. These self-evolving structures have numerous applications. For instance, these constructions can be put together without difficulty in deep water, which is difficult to achieve with other structures. Additionally, this might be useful while repairing items (ships, boats, etc.) in deep water. Instruments with such printable pieces that can be put together in a deep-water environment can also advance the exploration of deep-water bodies and plants. Such self-evolving 4D printed structures can also be utilized to improve the diving suit used by divers in deep water. Figure 16.1 shows different factors that are responsible for 4D printing.

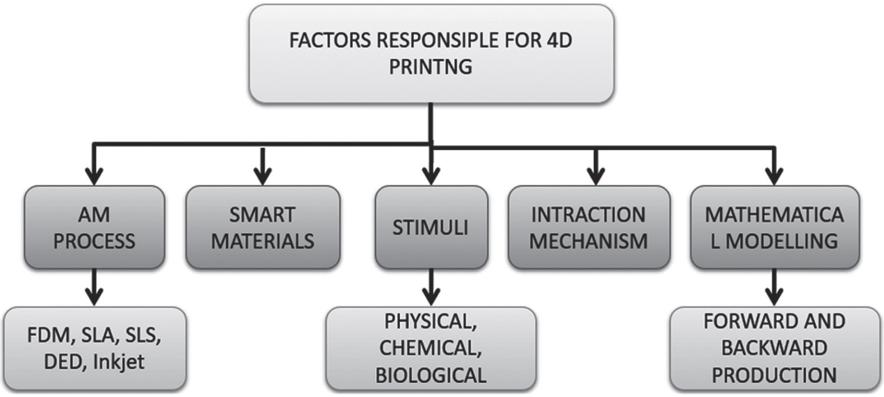
FACTORS RESPONSIPLE FOR 4D PRINTNG
AM PROCESS
SMART MATERIALS
STIMULI
INTRACTION MECHANISM
MATHEMATICA L MODELLING
FDM, SLA, SLS, DED, Inkjet
PHYSICAL, CHEMICAL, BIOLOGICAL
FORWARD AND BACKWARD PRODUCTION

FIGURE 16.1 Responsible factor for 4D printing. ⏎

16.4.4 APPLICATION AS ACTIVE ORIGAMI

A piece of paper is folded into a three-dimensional structure in the art of origami. The ability to shrink enormous items into small spaces is one of origami's key characteristics, which is being researched in today's modern world where it is necessary in many different industries. For instance, origami can be used to create cartons, shopping bags, auto-mobile airbags, and electronic devices (photovoltaic solar cells) where we need compact size and shape-changing properties. Since traditional origami can be expensive, the concept of active origami was created. Active origami, which is the creation of an origami structure with self-folding capabilities, calls for the use of SMs such as SMPs, light-activated polymers, etc. Since 4D-printed structures can self-fold and are simple and inexpensive to produce, they can be helpful in the development of active origami structures. Thus, the potential for active origami using multimaterials like PACs can be explored. Ge et al. used PACs hinge to create an active origami structure. In contrast to Ge et al. (who employed SMP in an elastomeric matrix), the authors of this work exclusively used SMPs as hinges for active origami. The benefit is that multimaterial SMPs offer a better active origami structure shape and design. Additionally, an active origami structure can respond to programming in either direction. The research team has created a variety of active origami structures, such as reconfigurable origami and multifolding origami, using this method and the appropriate changes.

16.4.5 APPLICATION IN AEROSPACE

Parts production for space missions is crucial to the aerospace industry. The components must be produced for less money and have a long lifespan. As was already said, 4D-printed structures can survive harsh environmental conditions and are made at a reasonable cost. Additionally, these structures are adaptable to their environment. As a result, the aerospace sector is discovering the potential applications of 4D printing. The eventual application of such materials in space missions has been suggested by the International Space Station's (ISS) 3DP of ABS constructions in microgravity. Additionally, they may be produced inside the spacecraft and have a short printing time, which lessens the need for components from Earth. The 4D structures can influence the course of such missions since they have the capacity to self-assemble in accordance with the circumstances. The shape memory alloy nitinol, which is composed of nickel and titanium, is extremely well-liked in the space industry and has been created utilizing 4D printing methods. The satellites, self-sustaining tools for space exploration, can be made in part from 4D materials. The light weight of structures created with 4D printing reduces a component's mass by 80%. PEEK, a thermoplastic that can withstand high temperatures and stresses with ease, has been printed using the SLS technology and is utilized to make parts for satellites and spacecraft. Figure 16.2 shows the material characteristics of 4D printing.

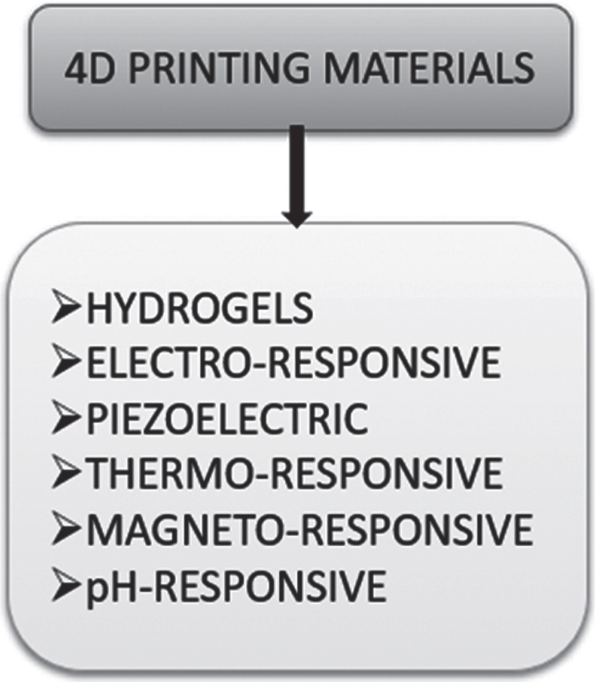

FIGURE 16.2 Characteristic of the material for 4D printing. ⏎

16.4.6 APPLICATION IN SENSORS AND FLEXIBLE ELECTRONICS

The creation of sensors can benefit from 4D printing. Due to the 4D printed structures' responsiveness to factors including pH, humidity, temperature, stress, and strain. For certain stimuli, they can therefore serve as sensors. Additionally, 4D printing is economical and produces lightweight, sensitive, accurate, and highly responsive structures. As a result, 4D printing will develop and modernize sensors. SMAs can be used to assess temperature, strain, and detect wear and damage inside a structure in addition to acting as actuators. Intelligent vehicles and aircraft can be produced using ultrasonic additive manufacturing (UAM), which mixes metals and SMs to print intelligent structures. UAM is a sort of 3DP that may be used to manufacture 4D structures and intelligent materials. UAM-printed structures have less mass, which is advantageous for the transportation sector. Construction mistakes can be fixed using 4D printing since the parts may be shipped to the defective area and self-assembled there with the application of the right stimulus. Self-healing structures can be created by utilizing the self-repairing capabilities of 4D-printed structures. The durability and dependability of the material systems will be improved by the self-healing materials using methylacrylate, where the framework was printed using SLA and the conductive ink was generated using inkjet printing. When heated above the melting point (T_m), the created structure was used to light an LED.

16.4.7 CHALLENGES AND FUTURE

A new field of study called 4D printing emerged along with 3DP technologies. The technology of 3DP is still in development. Since it is a relatively new field of study and is still in its infancy, 4D printing has several restrictions and difficulties that must be quickly resolved. Technology, material, and design issues are the three main problems with 4D printing. The lack of 3DP technology is one of the technological difficulties [29–31]. Only a few research institutions worldwide have access to 3D printers that can produce 4D structures. In the current situation, metallic and multimaterial components are printed utilising PolyJet and SLM printing methods, respectively. In contrast to SLM, which uses a laser to melt powder particles to print structures, PolyJet printers require that the material (smart) be in a liquid state in order for it to produce printed structures when exposed to UV light. Both instances require the SM to meet specific requirements; for PolyJet printing, it must be in a liquid form and responsive to UV light; for SLM printing, it must be in a powder condition. As a result, these printing methods would only be able to print a small number of SMs. a 4D print. The type and characteristics of the materials used for 4D printing present the following challenge. Since 4D structures are compositional sensitive, extra caution is needed to print structures without flaws when utilizing SMAs like NiTi. While some materials (hydrogels) decay with repetitive wetting and drying, some SMs can degrade with continuous deformation. Sometimes the substance has to be combined with other ingredients in order to make it printable. A hurdle for 4D printing is the combination of SMs with 3DP technology. In order to find novel SMs that can be printed directly, would not degrade over time, and work well with 3DP technology, more study is required. When made in a prestrain phase, smart structures can function as an actuator more effectively. However, only few works where such a prestrain mode has been accomplished have been recorded. Additionally, there is not a 3DP method that can print the prestrain membrane directly. Therefore, it is necessary to work on building smart structures for 4D printing. Additionally, the environmental effects of 4D printing have not yet been discussed; however, a report released in 2020 claimed that printing polymers in 4D can use 37.33% less energy. It was suggested that the temperature for form programming and recovery must be 10–15°C higher than the T_g. Future product manufacture and design will undergo a revolution once these limits are overcome by 4D printing. It will result in a new and effective business model by lowering the capital requirement, speeding up the marketing process, making products conveniently transportable, and shrinking their size. Because they can withstand extreme environmental conditions, 4D-printed structures can be used in space missions. As they can self-assemble, satellite and aircraft parts produced via 4D printing may be simple to assemble in space. Using structures that were printed in four dimensions, it would not be difficult to deform them in space. The design of 3D constructions can be made simpler with the use of 4D printing. With the use of 4D printing technology, user-responsive items that can respond to user needs can be produced. They can perform in accordance with user demands and adapt to their surroundings. Additionally, several intelligent materials that could develop 4D printing and expand its potential applications have not yet been fully investigated. New materials such as personalised textile composites, carbon fibers, and printed wood grain would expand 4D printing's capabilities. The primary focus of 4D printing's current applications is its capacity to change shape; however in the future, numerous other functionalities of 4D printed structures may be discovered, making them multifunctional. Future research on the varied responses of 4D-printed materials to stimuli is possible and will further its multifunctional applications. By the year 2025, 4D printing will reportedly have a global market worth of $537.8 million. Because 4D printing is a multidisciplinary area, future increased cooperation across its constituent fields will provide these structures more control over how they evolve in shape. Future developments in 4D printing will have a significant impact on how we live now.

KEYWORDS

- **4D printing**
- **additive manufacturing**
- **stereolithography**
- **directed energy deposition**
- **shape memory effect**
- **shape change effect**

REFERENCES

1. Hull, C., C. W., U.S. Patent 4575330, 1986.
2. Bower, C., Meitl, M., Gomez, D., Bonafede, S., Kneeburg, D. Inventors; X-Celeprint Ltd, assignee.. U.S. Patent 9358775, 2016).
3. Tofail, S.A., Koumoulos, E.P., Bandyopadhyay, A., Bose, S., O'Donoghue, L., Charitidis, C. *Mater. Today*, **2018**, *1*, 22.
4. Shirazi, S.F., Gharehkhani, S., Mehrali, M., Yarmand, H., Metselaar, H.S., Kadri, N.A., Osman, N.A. *Sci. Technol. Adv. Mater.*, **2015**, *3*, 16.
5. Choi, J., Kwon, O.C., Jo, W., Lee, H.J., Moon, M.-W. *Addit. Manuf.*, **2015**, *4*, 159.
6. Gao, W., Zhang, Y., Ramanujan, D., Ramani, K., Chen, Y., Williams, C.B., Wang, C.C., Shin, Y.C., Zhang, S., Zavattieri, P.D. *Comput. Aided Des.*, **2015**, *69*, 65.
7. Gibson, I., Rosen, D., Stucker, B., *Additive manufacturing technologies*. Springer: New York, NY, 2015.
8. Choong, Y.Y.C., Maleksaeedi, S., Eng, H., Yu, S., Wei, J., Su, P.C. *Appl. Mater. Today.*, **2020**, *18*, 100515.
9. Gu, G.X., Buehler, M.J. *Acta Mech.*, **2018**, *10,* 4033.
10. Nishiguchi, A., Zhang, H., Schweizerhof, S., Schulte, M.F., Mourran, A., Moller, M. *ACS Appl. Mater. Interfaces*, **2020** *12*(10), 12176–12185.
11. Libonati, F., Gu, G.X., Qin, Z., Vergani, L., Buehler, M.J. *Adv. Eng. Mater.*, **2016**, *8*, 1354.
12. Melchels, F.P.W., Domingos, M.A.N., Klein, T.J., Malda, J., Bartolo, P.J., Hutmacher, D.W. *Prog. Polym. Sci.*, **2012**, *8*, 1079.
13. Miyashita, S., Guitron, S., Ludersdorfer, M., Sung, C.R., Rus, D. In *Presented at IEEE International Conference of Robotics, Automation*, ICRA, May 2015.
14. Gaynor, A.T., Meisel, N.A., Williams, C.B., Guest, J.K. *J. Manuf. Sci. Eng.*, **2014**, *6*, 136.
15. Zegard, T., Paulino, G.H. *Struct. Multidiscip. Optim.*, **2016**, *1*, 175.
16. Gu, G.X., Chen, C.T., Buehler, M.J. *Extrem. Mech. Lett.*, **2018**, *18*, 19.
17. Gu, G.X., Chen, C.T., Richmond, D.J., Buehler, M.J. *Mater. Horizons*, **2018**, *939*.
18. Gu, G.X., Wettermark, S., Buehler, M.J., *Addit. Manuf.*, **2017**, *17*, 47.
19. Jared, B.H., Aguilo, M.A., Beghini, L.L., Boyce, B.L., Clark, B.W., Cook, A., Kaehr, B.J., Robbins, J. *Scripta Mater.*, **2017**, *135*, 141.

20. Hann, S.Y., Cui, H., Nowicki, M., Zhang, L.G. *Addit. Manuf.*, **2020**, *36*, 101567.
21. Compton, B.G., Lewis, J.A. *Adv. Mater.*, **2014**, *34*, 5930.
22. Wegst, U.G.K., Bai, H., Saiz, E., Tomsia, A.P., Ritchie, R.O. *Nat. Mater.*, **2015**, *1*, 23.
23. Gu, G.X., Libonati, F., Wettermark, S.D., Buehler, M.J. *J. Mech. Behav. Biomed. Mater.*, **2017**, *76*, 135.
24. Gu, G.X., Takaffoli, M., Buehler, M.J. *Adv. Mater.*, **2017**, *28*, 1.
25. Gu, G.X., Takaffoli, M., Hsieh, A.J., Buehler, M.J. *Extrem. Mech. Lett.*, **2016**, *9*, 317.
26. Hu, Y., Wang, Z., Jin, D., Zhang, C., Sun, R., Li, Z., Hu, K., Ni, J., Cai, Z., Pan, D., Wang, X., Zhu, W., Li, J., Wu, D., Zhang, L., Chu, J. *Adv. Funct. Mater.*, **2020**, *30*, 1907377.
27. Holmes, B., Zhu, W., Li, J., Lee, J.D., Zhang, L.G. *Tissue Eng.*, **2015**, *1–2*, 403.
28. Zhu, W., Holmes, B., Glazer, R.I., Zhang, L.G. *Nanomed. Nanotechnol. Biol. Med.*, **2016**, *1*, 69.
29. Firth, J., Gaisford, S., Basit, A.W. Springer: Cham, 2018, pp. 153–162.
30. Peppas, N.A., Hilt, J.Z., Khademhosseini, A., Langer, R. *Adv. Mater.*, **2006**, *11*, 1345.
31. Ge, Q., Qi, H.J., Dunn, M.L. *Appl. Phys. Lett.*, **2013**, *13*, 131901.

CHAPTER 17

SMART MATERIALS FOR HEALTHCARE

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ABSTRACT

Smart materials play a crucial role in various aspects of our lives, encompassing a wide range of sensing and actuation applications in healthcare due to their responsiveness to environmental stimuli. Research indicates that smart materials consistently exhibit greater biocompatibility than conventional stainless steel and other implant materials. The development of innovative nanostructured biomaterials and intelligent medical devices capable of perceiving, communicating, reacting to, and regulating their environment will be pivotal in the next generation of disease treatments. Nanomaterials are widely regarded as a potential tool for tumor detection, diagnosis, and treatment, with the utilization of smart materials in cancer treatment closely tied to advances in nanodrug delivery methods. The importance of hydrogels in a variety of life sciences is a result of their significant and useful 3D bio-polymeric networks. Hydrogels are interesting materials for the controlled release of medications. Recent developments in organic and polymer chemistry, bioengineering, and nanotechnology have led to a number of important improvements in the field of hydrogels for therapeutic delivery. In this chapter, we present our viewpoint on the state of the art in the field, concentrating on a number of fascinating themes.

17.1 INTRODUCTION

17.1.1 SMART MATERIALS

Intelligence in biological systems manifests as their capacity to interact adaptively with the environment. These systems, regardless of their complexity, can modify themselves in response to stimuli by utilizing information gathered from their surroundings. Likewise, the term “Smart” often describes materials that can reversibly change one or more of their functional or structural attributes in response to deliberate external stimuli or changes in their environment. These stimuli can be physical (like temperature, light, electric, or magnetic forces), chemical (such as pH or analyte concentrations), or mechanical (like stress or strain), all capable of inducing intelligent responses in materials. Importantly, this process should be entirely reversible, with smart materials returning to their original state once the trigger or external stimulus is removed. Notable examples of smart materials include shape memory alloys (SMAs) and polymers that adjust their physical properties, aiding actuation by regaining a predefined shape in response to temperature changes. Block copolymers with micro- or nanostructures can switch their surface characteristics from hydrophilic to hydrophobic (or vice versa) with temperature variations [1]. Additionally, piezoelectric materials can convert mechanical deformations into electric potentials and vice versa. Smart hydrogels, which expand and contract in response to pH changes, find frequent use in drug delivery systems. Some types of crosslinked polymers possess self-healing properties to repair mechanical damage. Furthermore, chemo-responsive polymer nanocomposites can alter their stiffness when exposed to specific chemical agents, resembling certain echinoderm structures. These examples underscore the significant potential of smart materials in the field of biomedicine.

Smart materials have garnered significant interest in the field of biomedicine due to their ability to modify certain properties in response to external stimuli or environmental changes. This chapter provides an introductory overview of smart materials and summarizes recent developments in biomedicine. The aim of this chapter is to acquaint the reader with the concept of smart materials before focusing on nanostructured piezoelectric materials in subsequent sections. We will briefly explore key categories of smart materials and provide examples of their applications in biomedicine [2].

Over the past few decades, there has been a growing fascination with scientific research and practical uses of microstructured advanced materials. The exploration of biomedical microdevices made from sophisticated materials has been particularly ignited by various factors. Discoveries of novel phenomena at the micro and nanoscales, along with advancements in processing technologies, have propelled nanoscience and nanotechnology into the spotlight, attracting a burgeoning community of researchers. In addition to the traditional audience of physicists, chemists, materials scientists, and engineers, biologists, and medical professionals have also begun showing interest in this research area, driven by the potential applications of micro and nanostructured materials. The evolving field of biomedicine demands increasingly advanced technical solutions to empower the latest generation of biomedical devices [3–5].

17.1.2 SHAPE MEMORY ALLOY

One category of smart materials, known as SMAs, consists of metallic materials that can alter their microstructure as needed. Smart materials in medical applications primarily rely on two effects: the shape memory effect and pseudo-elasticity. These effects involve two phases, austenite and martensite. Martensite, with its body-centered tetragonal structure, forms when austenite is rapidly cooled. Ni–Ti is a commonly used alloy in medical applications due to its suitability for achieving precise movements within the human body without causing harm. International organizations like the International Organization for Standardization and the American Society for Testing and Materials provide guidelines and standards for biomaterial production, testing, and the development of new materials [2] (Figure 17.1).

In recent years, cancer has remained the leading cause of death worldwide, presenting a significant ongoing health challenge. However, advancements in our understanding of tumor biology and more effective treatments have led to a decline in cancer mortality rates over the past few decades. While approaches like immune checkpoint inhibitors, gene-targeted therapy, and hormone therapy hold promise for improving outcomes, there is a need for novel drug delivery methods to overcome the limitations of traditional free medications [2–4].

Standard anticancer drugs, which have been in use for many years, suffer from issues such as low water solubility, nonspecific distribution in the body, severe toxicity to healthy cells, and the development of multidrug resistance. To address these shortcomings, drugs, like liposome paclitaxel and albumin paclitaxel, both nanomodified, have gained widespread adoption in oncology departments due to their high effectiveness and minimal side effects. This growing use of such medications has sparked interest among clinicians in nanodelivery devices, even though they may lack expertise in materials science. Providing clinicians with a user-friendly overview of nanodrug delivery is crucial to equip them with a foundational understanding of this field [6].

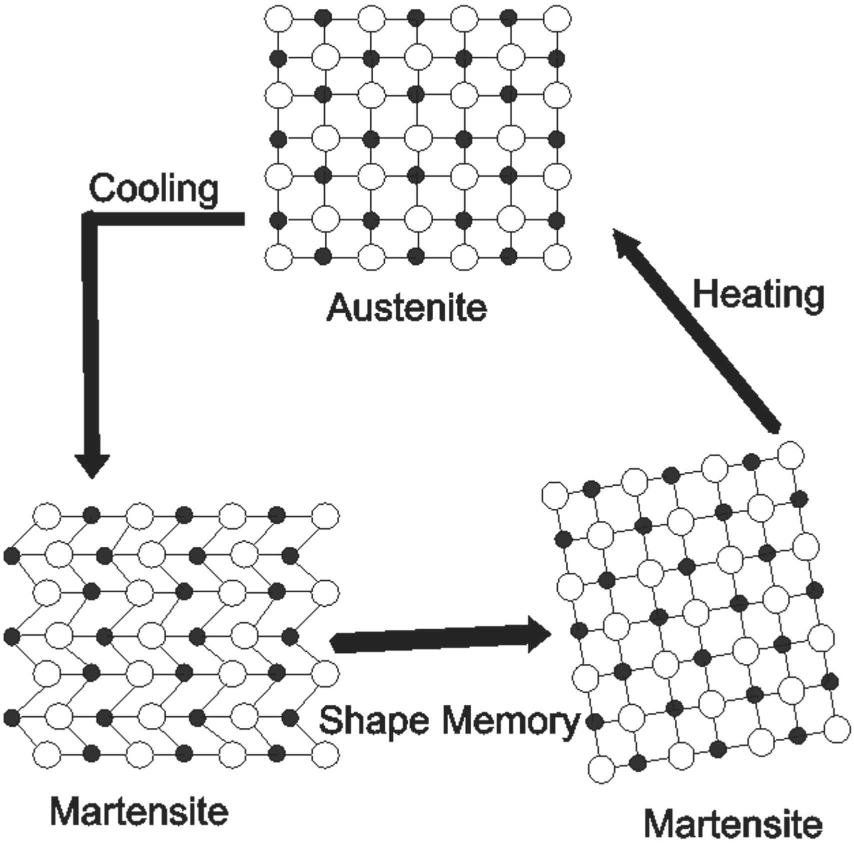

FIGURE 17.1 Two-way SMA. ⏎

17.1.3 HYDROGELS

Recent developments have elevated hydrogels to the status of noteworthy carrier substances, and they have distinguished use in the administration of drugs to tumors. Because it is known to be an effective delivery agent at particular tumor sites and has fewer adverse effects than the current systemic chemotherapy. Additionally, it has notable qualities including being less hazardous than nanoparticle carriers and being biocompatible and biodegradable. This has opened the door for researchers to go deeper and look more closely at how hydrogels function. *In-situ* gelations and controlled release of drugs are made possible by smart hydrogels, which can react to environmental stimuli including heat, pH, light, and ultrasound. This dramatically improves the ease and effectiveness of drug delivery [12]. The production of hydrogels is caused by repeated monomers, such as homopolymers or copolymers, which contain hydrophilic polymer chains and are organized in various ways.

Hydrogels are effective drug delivery vehicles, and their usage in clinical settings has significantly improved treatment outcomes. Improvements have been made in the spatial and temporal delivery of cells, small molecules, and macromolecular medicines in hydrogel encapsulation. The limitations of the hydrogel drug delivery design have been partially solved, and this has led to the development of an improved carrier [13].

Particularly for the administration of macromolecules and hydrodynamic drug molecules, hydrogels have the potential to be effective in delivering drugs through the mouth. As a result, the use of hydrogels in the treatment of diabetics and cancer patients has been expanded. With oral drug administration, the drug is specifically administered to the mouth, stomach, small intestine, as well as colon. For this use, muco-adhesive hydrogels are typically employed. Due to their powerful effects and excellent selectivity, protein and peptide medications are becoming more and more important nowadays. However, the enzymatic activity in the GI tract, which causes the degradation of these pharmaceuticals, poses a serious challenge. Hydrogels have a crucial role in the administration of protein and peptide medications across the GI tract, according to studies, which have demonstrated that they provide a platform that helps to deliver the drugs to specific areas in the GI tract [14] (Figure 17.2).

17.1.4 WHY SMART MATERIALS IN BIOMEDICAL APPLICATION?

Smart materials have found application in microtechnology to achieve novel capabilities in microscopic devices, including sensing abilities. This usage is evident in the creation of microelectromechanical systems and nano electromechanical systems devices [7]. Moreover, they have the potential to enable advanced methods for energizing and controlling the movement of minuscule objects. In the context of these microscale applications, it is essential to precisely customize the physical and chemical properties and capabilities of smart materials. Often, they must exhibit adaptability to diverse operational conditions and manufacturing techniques.

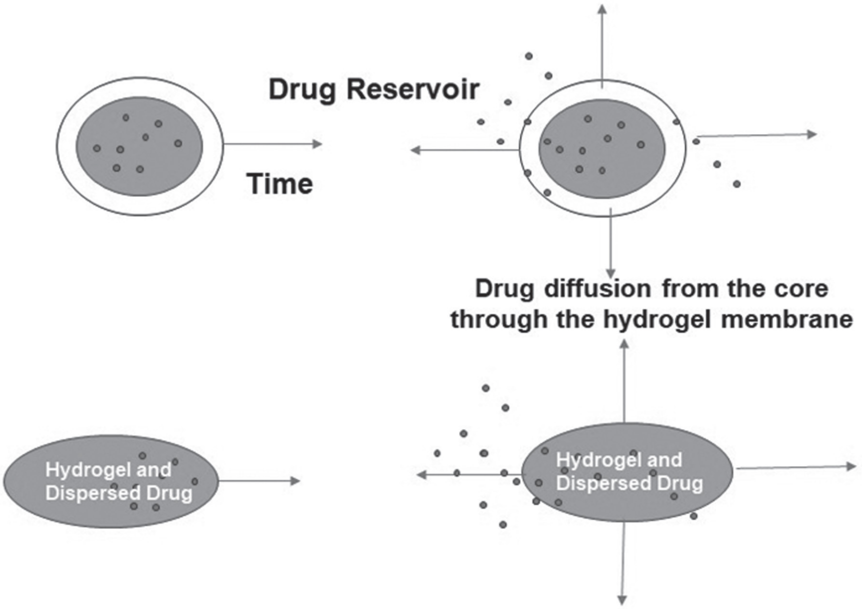
Drug Reservoir
Time
Drug diffusion from the core through the hydrogel membrane
Hydrogel and Dispersed Drug
Hydrogel and Dispersed Drug

FIGURE 17.2 A hydrogel membrane and matrix administration enables drug dissolution. ⏎

17.2 PREPARATION OF SMART MATERIALS

The alloys predominantly employed in medical applications include Ni–Ti and SE Ni–Ti. These alloys are crafted through either a vacuum induction melting process or a double vacuum melting method. These distinct techniques are employed to produce SMAs while ensuring a low level of impurities in the alloy and achieving proper alloy integration. The molten metal is rapidly cooled by either water or the surrounding air, resulting in a solid block of pure metal with a trapezoidal cross-section. To attain the desired characteristics and flexibility for various product sizes and shapes, a double-melted ingot undergoes hot and cold working. The alloys are heated to a precise temperature, allowing for the reordering of dislocations in a predetermined manner without inducing re-crystallization. Following this, they are shaped while still hot and promptly cooled using water or ambient air.

17.3 PROPERTIES OF SMART MATERIALS

Smart materials can change their properties in response to external elements including light, temperature, moisture, stress, magnetic or electric fields, or chemical substances in a regulated manner. These are referred to as responsive materials. The constituent materials and chemical makeup of natural systems possess the capability to sense their environment, process information, and respond promptly. Smart materials exhibit mechanical properties that encompass self-correction, self-regulation, self-repair, sensing abilities, shock absorption, super elasticity, compatibility with biological systems, compactness, safety mechanisms, and more. These unique characteristics distinguish smart materials from traditional implantable devices, making them valuable assets in the biomedical sector. When an external force is supplied, smart materials alter:

1) Thermo-chromic ink transforms its color when heated.
2) When electricity flows through electroluminescent materials, they shine.
3) Photo-chromic ink transforms when exposed to UV light.
4) Electrical currents can be run through conductive ink.

17.4 MEDICAL APPLICATIONS OF SMART MATERIALS

Applications for smart materials are expanding across various industries. The following are the uses of smart materials in the medical field

1) Angioplasty
2) Cardiovascular
3) Orthopedic
4) Orthodontic

17.4.1 ANGIOPLASTY

An artery with plaque buildup can be made larger inside the artery via a treatment called angioplasty. In order to push plaque against the artery walls and allow blood to flow through artery, healthcare practitioner will use a tiny balloon. They frequently also insert a stent or tube to maintain the newly created opening. Smart materials contain inherent qualities that adapt in a regulated way to outside stimuli. SMAs, particularly Nitinol, are currently the only intelligent materials with a major therapeutic impact on cardiovascular implant design.

The intra-aortic balloon pump is employed to remove an abnormal fatty buildup within a blood artery. These tools need to possess flexibility and should not adversely affect human tissue since they are inserted into the body. Consequently, they feature a smaller diameter compared to polymer-based materials. Furthermore, they offer greater reliability and enhanced resistance to torsion when compared to stainless steel tubes and other implantable devices (Figure 17.3).

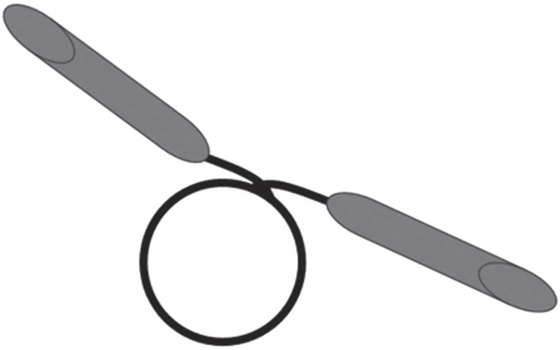

FIGURE 17.3 Vascular balloon pump. ⏎

17.4.2 CARDIOVASCULAR

The intricate cardiac vasculature needs robust, long-lasting, yet delicate cardiovascular therapy. The cardiovascular system's complex network of arteries and sensitive endothelial surfaces call for streamlined internal movement and manipulation. Nonthrombogenic surface chemistry is necessary for cardiovascular devices implanted in blood to prevent clot and blockage formation.

The circulatory system, encompassing the heart and blood vessels, is part of the cardiovascular system. It incorporates wires made from SMA and a waterproof polyurethane coating. The implantation procedure for the Simon filter, which utilizes the shape memory effect, is considerably less invasive than the traditional approach. A catheter is used to introduce one-half of the Simon filter in its folded state through the vena cava to the heart. It is then positioned over the atrial opening, unfolded, and returned to its original shape. This process is repeated to attach the second half of the Simon filter, effectively sealing the hole in the blood vessel and preventing blood flow between the atria. As heart tissue regenerates, the Simon filter can remain within the body indefinitely. Additionally, this device finds application in various scenarios to support various tubular structures, including bile ducts and blood vessels such as the coronary, iliac, and aortic (Figure 17.4).

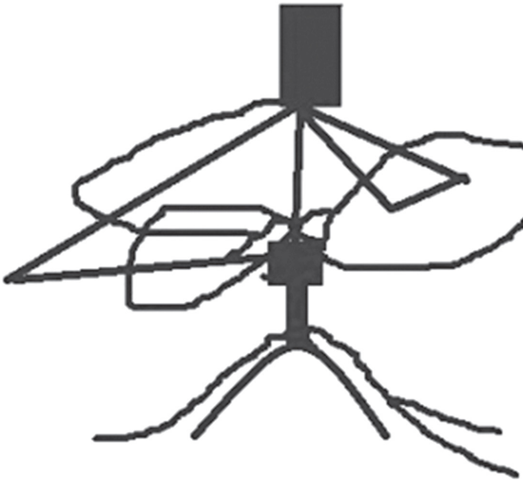

FIGURE 17.4 Simon Haul. ⏎

17.4.3 ORTHOPEDIC

SMA is predominantly utilized in various applications related to joints and the muscular system. When mending a broken bone, shape memory staples are placed in their open configuration at the desired location. As the wound heals, these staples typically close, bringing together the fractured or separated bone segments. External heating is applied to activate the staple; it does not rely on the body's natural temperature. These staples, along with fracture screws and other methods, are employed to maintain the bone's natural alignment and encourage cellular regeneration. The shape memory effect, which aids in regaining their original form and reuniting fractured segments, contributes to the healing process. Once smart materials are introduced in the fracture area, these SMA alloy wires facilitate the restoration of natural movement by mimicking the function of hand muscles [8, 9] (Figure 17.5).

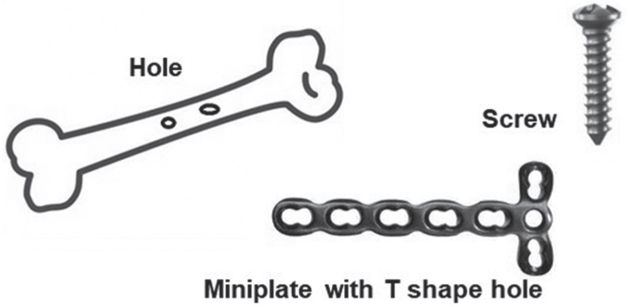
Hole
Screw
Miniplate with T shape hole

FIGURE 17.5 Applications in orthopedics. ⏎

17.4.4 ORTHODONTIC

Biocompatibility of a smart material essentially refers to its ability to be well-received by the body. This is crucial because the introduction of any foreign substance into either soft or hard tissue can trigger a foreign body reaction. Ni–Ti alloy, which has been employed in orthodontics for many years, has proven to be well-tolerated by patients in its cold-wrought martensite state. Smart materials find use in a range of applications, including clips, self-expanding and highly elastic nitinol stents, as well as staples (Figure 17.6).

FIGURE 17.6 Applications for nitinol wires in orthodontics. ⏎

17.5 SMART MATERIALS FOR HEALTHCARE

The development of innovative nanostructured biomaterials and intelligent medical devices capable of sensing, communicating, responding to, and regulating their surroundings holds significant importance for the future of disease treatments. Progress in new biomaterials, nanotechnology-based manufacturing methods, and enhanced understanding and control of the chemistry, physics, and biology at the interface between these devices and body tissues will all play a pivotal role in advancing healthcare.

Furthermore, emerging biomaterial technologies will address several existing medical challenges associated with current devices, such as issues related to tissue compatibility, corrosion, device-related infections, and nonspecific organ toxicity. To ensure the ongoing safety and efficacy of medical devices and to gain a deeper understanding of how these biomaterials and devices function within the body, it is imperative to comprehend their interactions with the human body.

Smart biomaterials possess the remarkable ability to sense their environment and modify their properties, such as shape, solubility, orientation, or phase, to achieve desired medical outcomes. Biomaterials, in general, encompass substances used to repair, replace, or enhance human tissues, structures, and systems, and some of them possess environmental sensing capabilities. These intelligent biomaterials often feature nanoscale structures and exhibit self-healing properties, adapting to changes in conditions like temperature, pH, electrical currents, and fields, among others. Examples include preventing microbial adherence while promoting host cell growth and releasing therapeutic drugs in response to specific triggers like the altered pH of tumors or inflamed tissues. Smart materials can also be designed for precise drug delivery to specific locations within the body. Smart scaffolds, utilizing advanced materials to mimic natural development, homeostasis, or healing processes, hold promise for biomimetic tissue engineering of organs and tissues. In healthcare, these materials can enhance medical device functionality by promoting favorable biological responses such as tissue growth and healing.

Syracuse Biomaterials Institute has initiated research programs in various areas such as shape memory polymers for medical devices, polymer coatings, metallic biomaterials' *in vivo* performance, biomaterial surfaces, bone cements, interactions between biomaterials and bacteria, tissue engineering, and mechano-biology. This focus area will be further developed and expanded, with an emphasis on clinical testing to understand organism reactions to implants and surface studies aimed at improving the functionality of medical implants.

17.5.1 SMART MATERIALS APPLIED IN CANCER THERAPY

17.5.1.1 CANCER TREATMENT

Despite the extensive use of traditional cancer treatments for over five decades, they have not yielded satisfactory results. Smart materials offer the potential to extend the duration of drug circulation, reduce off-target toxicity, and enhance the stability and solubility of enclosed medications. Additionally, the versatile design capabilities of smart materials make them attractive as multifaceted nanocarriers. Over time, smart materials have introduced several innovative cancer therapy options like Doxil, Abraxane, Vyxeos, Onpattro, and others. Beyond these commonly used chemotherapy drugs, nanotechnology has been explored for applications in immunotherapy, molecular targeted therapy, radiation therapy, phototherapy, and more. While only a fraction of nanoparticles (NPs) will ultimately see practical use, nanotechnology is expected to pave the way for new approaches to diagnosing, treating, and preventing tumors.

17.5.1.2 CHEMOTHERAPY

Although traditional chemotherapy has limitations due to off-target effects and the development of adaptive resistance, it remains a common cancer treatment. The outlook is expected to improve with the advancement of smart materials for chemotherapeutic drug delivery. Smart materials in drug delivery systems have the potential to enhance the distribution of chemotherapeutic drugs, reduce their toxicity, and overcome drug resistance.

Doxil, the first FDA-approved liposome-based chemotherapeutic drug, is an example. It utilizes Pegylated liposomal doxorubicin modified with PEG on the liposome's surface, resulting in prolonged circulation and half-life in the bloodstream and selective tumor targeting in clinical applications. Human serum albumin, a major serum component, has been extensively studied as a drug carrier for chemotherapy [9]. Abraxane, considered a significant clinical success, has been shown to extend patient survival by an average of 2.76 months. It eliminates life-threatening hypersensitivity and severe allergic reactions associated with polyoxymethylene castor oil. Administration is simplified as corticosteroids are not needed to prevent hypersensitivity reactions. Drug resistance poses a challenge to immune checkpoint inhibitors and traditional chemotherapy drugs, limiting their effectiveness.

The smart materials drug delivery system introduces an alternative approach to drug penetration into cells, potentially bypassing the action of multidrug resistance transporters responsible for expelling anticancer drugs from cancer cells and causing multidrug resistance. One well-known drug resistance mechanism is P-glycoprotein. Research suggests that NPs may overcome P-glycoprotein-mediated resistance, possibly because NPs, upon entering cells, are encapsulated in endosomes, evading detection by the P-glycoprotein efflux pump. Ligand-targeted NPs, particularly those coated with receptor-targeting ligands, can enhance drug delivery to cells, increasing intracellular bioavailability [8] (Figure 17.7).

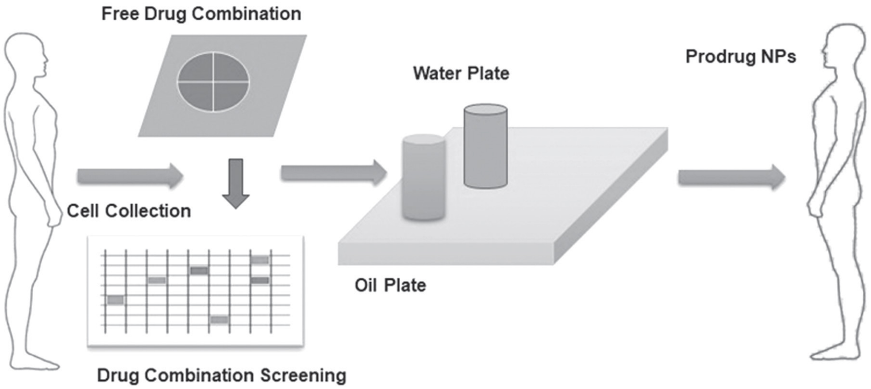

FIGURE 17.7 Method of drug delivery. ⏎

17.5.1.3 TARGET TREATMENT

Molecular targeted therapy is a widely embraced approach in medical oncology that can significantly extend the survival and improve the quality of life for cancer patients. One of the most prevalent driver mutations in cancer involves the activation of tyrosine kinase receptor proteins, and abnormal alterations in these receptors and their downstream pathways play a pivotal role in the development of various tumors. Tyrosine kinase receptor inhibitors, the most commonly utilized molecular targeted drugs, have seen extensive clinical use.

17.5.1.4 RADIOTHERAPY

Radiotherapy is a widely used and effective treatment for alleviating symptoms caused by tumor compression and pain. It also serves as a curative option for some patients. Despite its widespread use, there remain areas where improvements are needed, including strict dose limits for specific sites, challenges in continuing radiotherapy after radical treatment, and the risk of inaccuracies in radiation that can harm healthy tissues.

One fundamental strategy to enhance the effectiveness of tumor radiation therapy involves the use of radiosensitizers. When a radiosensitizer is present, even a low radiation dose can positively impact tumor treatment. Nanomaterials offer a wide range of potential applications in radiation therapy. For instance, the effectiveness of radiotherapy is closely linked to the oxygen levels within the tumor site. Ensuring sufficient oxygen at the tumor site can delay the repair of DNA damage, thus enhancing the efficacy of radiotherapy. Since many tumor locations exhibit hypoxia, addressing this oxygen deficiency is critical to improving radiotherapy outcomes.

17.5.1.5 PHOTOTHERAPY

Phototherapy is a noninvasive treatment approach that combines phototherapeutic drugs with light irradiation. It has the potential to selectively destroy cancer cells while minimizing harm to healthy cells when conducted in the absence of light. Achieving precise control over when and where light is applied is essential in phototherapy. Typically, light is administered only when the drugs have reached the tumor sites, ensuring temporal and spatial accuracy. Conversely, controlling external light exposure can help mitigate the side effects associated with the continuous release of drugs. Phototherapy comes in two fundamental forms: photothermal therapy and photodynamic therapy.

17.5.1.6 FURTHER THERAPY

In addition to the commonly employed modalities in clinical settings, there are other important therapeutic approaches in nano-antitumor therapy. These include chemo dynamic treatment, electrodynamics therapy, and acoustic therapy. While these methods may not be widely utilized in clinical practice, they have demonstrated success in cellular and animal studies, suggesting their potential for broader application. Therefore, it is essential for oncologists to have an understanding of these therapies. This knowledge not only provides new insights into the utilization of nanodrugs in oncology but also expands the horizons of anticancer treatment possibilities [9].

17.5.2 HYDROGEL-BASED TARGETED DRUG DELIVERY

The crosslinking polymeric materials known as “hydrogels” have been playing important roles in a variety of fields. Hydrogels are crosslinked, three-dimensional (3D), insoluble polymer networks that resemble tissues and can hold a lot of water and biological fluids when they're swelled. Chain networks expand as a result of capillary, osmotic, and hydration pressures that interact with polymeric chain networks and aqueous or biological liquids and are counterbalanced. Internal transport, diffusion properties, and mechanical strength are only a few of the fundamental qualities of the hydrogel that are determined by its equilibrium state, which is dependent on the strength of these opposing processes [11].

Researchers have outlined hydrogels in a variety of methods over the years. The most popular definition states that a hydrogel is a crosslinked polymeric network that is water-swollen and created by the straightforward reaction of a single monomer, polymer, and crosslinker units. Another way to describe it is that it is a polymeric substance that can absorb a lot of water and hold it in its three-dimensional network without dissolving. They can also be described as polymeric structures that exhibit the ability to expand in the presence of water and hold onto a sizeable amount of that water within their 3D structure without disintegrating. Food and biological material scientists refer to polymers with crosslinked network structures as gels or hydrogels interchangeably. According to their flow behavior in steady-state, gels are classified primarily as either strong or weak systems that are extensively diluted in crosslinking [10].

17.5.2.1 SUPRAMOLECULAR HYDROGEL

As an alternative to artificial polymers for the delivery of drugs, supramolecular hydrogels made from peptides, proteins, and other biomaterials have lately gained popularity. Self-assembled peptides are a potential class of supramolecular gelators for the *in vivo* delivery of drugs that have been slow to catch on despite gains in biocompatibility because synthetic peptide hydrogels are more expensive than synthetic polymer gels. The superior biocompatibility of supramolecular hydrogels and ease of formulation compared to polymer hydrogels have led to research into the self-assembly processes that cause the gelation as well as how to engineer the novel characteristics of supramolecular gels to produce superior delivery systems for medicinal materials. Researchers have become interested in the creation of stimuli-responsive hydrogels for medicine administration.

The noncovalent interactions between molecules make up the supramolecular hydrogel structure, which holds two or more molecular units collectively. Because it avoids the difficulties of constrained loaded drug ability and drug inclusion for use exclusively as implants, which can be the only choice with a covalent crosslinked system, the noncovalent crosslinked nature of these hydrogels serves as a particularly desirable feature. These hydrogels not only give the hydrogels the essential physical stability but also allow for simultaneous loading of drugs and gelation in aqueous circumstances without the use of covalent crosslinking processes.

Supramolecular hydrogels that respond to biological triggers have attracted a lot of attention recently due to their potential as intelligent materials. For example, a stimulus-triggered gel-to-sol phase transition may be a macroscopic sensor. A drug-encapsulated supramolecular hydrogel could administer the medication according to the stimuli-responsive gel-to-sol phase change. To take advantage of the benefits, however, supra molecular hydrogels that exhibit a gel-to-sol phase shift in responses to biological stimulus must be created in physiological conditions.

17.5.2.2 MULTICOMPONENT HYDROGEL

One common example of the adaptability of these delivery mechanisms and their susceptibility to chemical alterations to increase their therapeutic effects is the multifunctional hydrogels that serve as carriers of anticancer medications. The materials are promising materials for biological uses such as drug administration, wound repair, and tissue engineering due to their exceptional cytocompatibility and biocompatibility. However, it is possible to overlook the possibility of toxicity of products from breakdown while choosing materials. For instance, the well-liked breast implant amazingly is nontoxic and has a low likelihood of rejection.

For use in medical applications, hydrogels and their breakdown products' biocompatibility must be investigated. Material quality may be improved by the development of novel, reasonably priced biomimetic substances or organic substances obtained through high-volume processing methods, such as hyaluronic acids, chitosan-based gelatin, collagen, and others. As a class of smart materials, stimuli-responsive hydrogels hold potential for customized drug delivery. Due to a complex design, its hydrogel frameworks can be automatically activated in response to pathological surroundings and deliver cargos with improved spatial/temporal resolution.

Inadequate drug distribution in solid tumors can also result in resistance to drugs and a sharp decline in therapeutic effectiveness. Drug-encapsulated hydrogel capsules that respond to target biomarkers may improve this sector. Thanks to the change of aptamers, molecules that specifically target particular cells, hydrogel capsules with excellent specificity and permeability offer a fresh perspective on cancer therapy. Another interesting approach for overcoming the issues mentioned above and enhancing therapeutic outcomes is the use of multiple-triggered hydrogels with programmed functionality.

17.5.2.3 DNA-BASED HYDROGELS

The following traits of DNA-based hydrogels are distinctive: biodegradability, absence of immunity, a high degree of sensitivity, and delivery of drugs. The Watson–Crick base pairing principle governs the self-assembly of biomaterials, which is how DNA hydrogels are created. DNA is an appropriate substance for the building of hydrogels with adjustable mechanical characteristics and formulation that might find application in several biological fields, such as designing of novel multifunctional biomaterials, due to its special mechanical and biochemical features as well as its biocompatibility.

A drug carrier is successful if it possesses properties including maintaining the bioactivity of the medications intact, preventing chemical and enzyme degradation, and improving retention. DNA hydrogel was elevated by its advantageous traits, including biocompatibility, cargo availability, stimuli responsiveness that is simply activated, and effective active targeting capability. Molecules of drugs and NPs of inorganic material can be integrated into the porous structural networks with a low loading efficiency [14].

17.5.2.4 STIMULI-RESPONSIVE HYDROGELS

Hydrogels that are stimuli-responsive are classified as important subgroups because they alter their structural or mechanical characteristics in response to environmental cues or triggers. These hydrogels are extremely useful in the biological and robotics domains. There are many stimuli that can be used to induce a phase transition or rigidity change in these materials, including temperatures, light, magnetic fields, electric fields, pH, chemicals, and biological triggers. This suggests that these materials have an abundance of uses in division, delivery of drugs, sensing, bionic gadgets, regenerative healthcare, and more. Attention has been drawn to two categories of bio-stimuli for the creation of bio-functional materials: endogenous stimuli, which are present naturally in the bio-environment, and external biocompatible stimuli, which activate the hydrogel system’s smart functions. Endogenous stimuli include things like pH level, ions of metal, digestive enzymes, redox atmosphere, antigens, and other things. The exocellular pH of tumor tissues is lower than that of normal tissues due to inappropriate metabolism, particularly glycolysis overactivity, and lung cancer cells have a specific protein that could be recognized by antibody-functionalized microgels. Reactive oxygen species are produced in wounds or bacterial infections, for example, creating an oxidative environment (Figure 17.8).

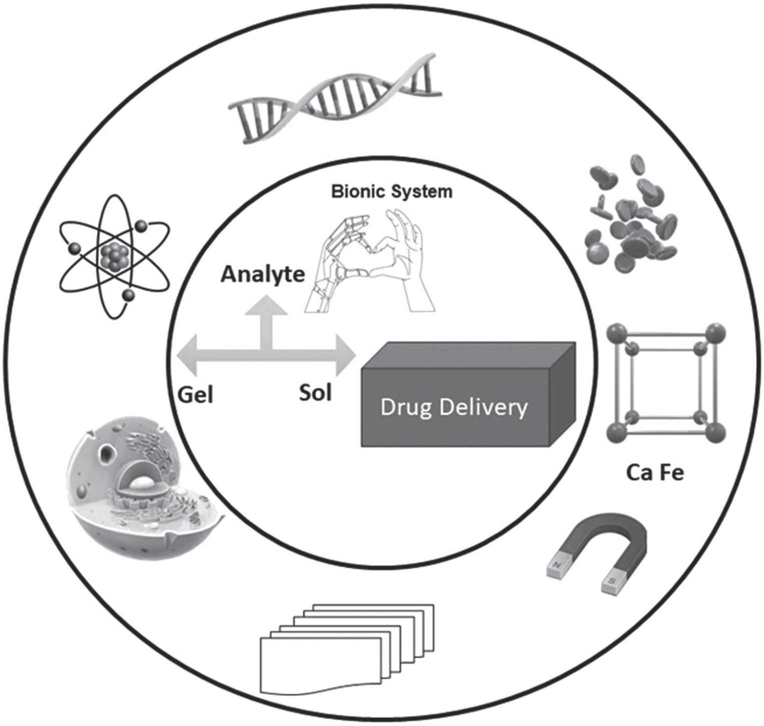

FIGURE 17.8 Hydrogels that respond to stimuli and uses. ⏎

17.5.2.5 CHALLENGES OF HYDROGEL DRUG DELIVERY

How to load a hydrophobic drug to the matrix of gel and, once active, how to efficiently transfer the drug into the water-based gel surroundings are the two main challenges in hydrophobic drug delivery. Hydrophobic medication loading into hydrogels has been improved by the use of a number of techniques. The biological barrier concerns are related to problems with systemic drug distribution, whereas the physiochemical obstacles are brought on by low solubility in water, the elevated molecular weight of therapeutic peptides and proteins, and challenges in producing controllable drug release.

17.5.3 NANOGEL

The new horizon in biology and medicine is represented by nanostructures made up of medicinal molecules with novel architectures. Figure 17.9 illustrates the use of nanogel in many biological fields. Nanogels are crosslinked polymer networks with a 3D framework and a range of nanoscale sizes. Although these nanogels may store a lot of water, they would not dissolve in aqueous solutions. They frequently have a spherical shape, but their synthetic processes might vary. Researchers recently discovered nanogels, which have been used as a promising tool to address the crucial problems associated with intracellular delivery. Because of their peculiar characteristics, such as swelling behavioral characteristics, nanogels may cross the membrane of a cell and release their cargo in the cytoplasm without inciting an immune response. These can be produced using either synthetic or naturally occurring polymers, or a combination of the two. The chemical makeup of nanogels can change their distinctive properties [17].

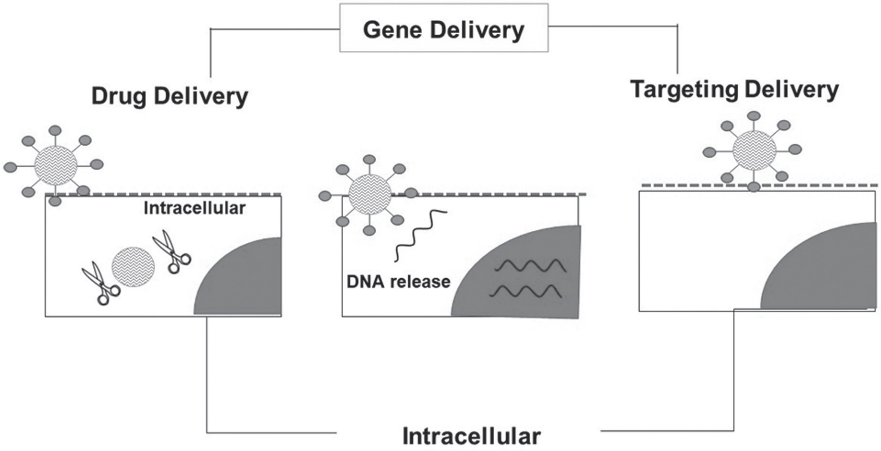

FIGURE 17.9 Diagram showing nanogels used in different biological applications. ⏎

They are at the forefront of the delivery of drugs and delivery of genes due to their characteristics including swelling and encapsulation as well as the previous reaction in the specifically selected regions. There are two ways to create the nanosized gel: top-down and bottom-up. Different methods are known to produce NPs from big clusters of particles in a top-down manner. This method's limitations may be caused by the defects in particle surfaces. The bottom-up technique can be used to create and arrange molecules by direct polymerization of monomers and the assembly of polymer precursors through bonding [15–17]. Nanogels' size distribution and stability are crucial in biomedical applications. The chemical makeup of the matrix of polymer and the type of crosslinking used in the polymer chains both affect stability. Physically crossed-linked nanogels are weaker and less stable than chemically crosslinked nanogels; however, chemically crosslinked nanogels are far more appealing because of their long-term stability and reproducibility [18]. Proteins, peptides, nucleic acids, medicines, fluorophores, and other small nanosized particles can all be incorporated into nanogels. Both the nanogel and nanostructured gels have the capacity to encapsulate several compounds.

17.6 CONCLUSIONS

In competitive fields like automotive manufacturing, robotics, eyewear production, and thermostat manufacturing, smart materials have a distinct advantage due to their biocompatibility, reliability, and resistance to corrosion. SMAs particularly excel in sensing and responding compared to other materials, making them successful in biomedical applications where they operate safely within the human body. Their unique characteristics make SMAs particularly stand out in the biomedical sector, setting them apart as valuable and purpose-driven materials.

Smart materials possess essential attributes such as being significant, measurable, goal-oriented, and adaptable, setting them apart from conventional models. Consequently, SMAs find relevance in a wide array of applications, with growing importance in engineering, medical technology, and aviation in the years to come. While the use of smart materials in cancer therapy shows promise in revolutionizing drug administration and delivery of anti-tumor medications, there is room for improvement in terms of biocompatibility, clinical outcomes, and safety. The dynamic nature of the internal environment within the human body adds complexity to this endeavor. Continued research into mechanisms that differentiate between tumor and normal tissues will likely lead to more targeted drug delivery. Smart materials have the potential to serve as efficient drug carrier systems, delivering positive patient outcomes. They possess controlled release mechanisms that enable selective destruction of tumor cells while minimizing harm to healthy cells, and their ability to penetrate bodily barriers efficiently is particularly valuable. Achieving success with smart materials in cancer treatment largely hinges on effective nanodrug delivery methods.

There are many benefits of using hydrogels for targeted drug delivery, including biocompatibility, minimal toxicity, and optimal swelling behavior. Depending on the chemical components of the gel-forming polymers and the route of administration, there have been some challenges in the processing of hydrogels. These challenges include some restrictions in the delivery of active pharmaceuticals, such as slow stimuli-sensitive hydrogel responsiveness, the potential for rapid burst drug release, the potential for drug regeneration, limited hydrophobic nature of drug delivery, and low mechanical durability. As a result, the area of nanoscience is positively influencing the development of intelligent hydrogel compositions that can mimic tissues by altering their swelling and nonswelling processes, which directly affects their ability to function as intelligent carriers in the pharmaceutical discipline.

KEYWORDS

- **smart materials**
- **electric field**
- **magnetic field**
- **nanostructured biomaterials**
- **hydrogel**
- **nanogel**
- **drug delivery**
- **cancer treatment**

REFERENCES

1. Darrel, E., Hodgson, H., Ming, H. *Shape memory alloys: nonferrous alloys and special-purpose materials, properties and selection*. ASM Handbook, 2010, pp. 897–902.
2. Dai, K., Chu, Y. *Biomed. Mater. Eng.*, **1996**, 233–240.
3. Andreasen, G.F., Edie, J.W., Zaytoun, M.P. Nitinol and stainless steel surface corrosion in a clinical setting. **1981**, 319–324.

4. Anoop, K.R., Honey Priya, J., Rijo, J., Anju, A. A brief summary of smart polymers for the controlled distribution of pharmaceuticals. *Acta Pharm. Sin. B*, **2014**, 120–127.
5. Machado, L.G., Savi, M.A. Medicinal uses of shape memory alloys. *Brazilian J. Med. Biol. Res.*, **2003**, 683–691.
6. Lopez-Soto, A., Gonzalez, S., Smyth, M.J., Galluzzi, L. NK cells regulate metastasis in cancer cell. *Cancer Cell*, **2017**, *32*(2), 135–154.
7. Bray, F., Ferlay, J., Soerjomataram, R.L., Siegel, L.A., Torre, Jemal, A. World cancer statistics. *CA Cancer J. Clin.*, **2018,** *68*(6), 394–424.
8. Duerig, T.M., Pelton, A., Stöckel, D. An overview of nitinol medical applications. *Mater. Sci. Eng.*, **1999**, *149–160*, 273–275.
9. Mantovani, D. Shape memory alloys, properties and biomedical applications. *J. Miner. Met. Mater. Soc.*, **2000**, 36–44.
10. Honey Priya, J., Rijo, J., Anju, A., Anoop, K.R. Smart polymers for the controlled delivery of drugs—a concise overview. *Acta Pharm. Sin. B.*, **2014**, 120–127.
11. Cabane, E., Zhang, X., Langowska, K., Palivan, C.G., Meier, W. Stimuli-responsive polymers and their applications in nanomedicine. *Biointerphases*, **2012**, *9*, https://doi.org/10.1007/s13758-011-0009-3
12. Otto, S., Marina, P.F., Zhou, F., Blencowe, A. Thermoresponsive polysaccharides with tunable thermoresponsive properties via functionalisation with alkylamide groups. *Carbohydr. Polym.*, **2021**, 254, https://doi.org/10.1016/j.carbpol.2020.117280
13. Das, D., Ghosh, P., Ghosh, A., Haldar, C., Dhara, S., Panda, A.B., Pal, S. Stimulus-responsive, biodegradable, biocompatible, covalently cross-linked hydrogel based on dextrin and poly for in vitro/in vivo controlled drug release. *ACS Appl. Mater. Interf.*, **2015**, 14338–14351.
14. Lin, F., Zheng, J., Guo, W., Zhu, Z., Wang, Z., Dong, B., Lin, C., Huang, B., Lu, B. Smart cellulose-derived magnetic hydrogel with rapid swelling and deswelling properties for remotely controlled drug release. *Cellulose*, **2019**, 6861–6877.
15. Narayanaswamy, R., Torchilin, V.P. Hydrogels and their applications in targeted drug delivery molecules. *Molecules*, *24*(3), **2019.**
16. Li, Z., Zhou, Y., Li, T., Zhang, J., Tian, H. Stimuli-responsive hydrogels: fabrication and biomedical applications. *VIEW*, **2021**, *3*(2). doi: 10.1002/VIW.20200112.
17. Mauri, E., Perale, G., Rossi, F. Nanogel functionalization: a versatile approach to meet the challenges of drug and gene delivery. *ACS Appl. Nano Mater.*, **2018**, 6525–6541.
18. Labhasetwar, V., Leslie Pelecky, D. *Biomedical Applications of Nanotechnology*, Wiley-Interscience, 2007, p. 264.

CHAPTER 18

BINARY CHALCOGENIDE POLYMER NANOCOMPOSITES FOR ELECTROLUMINESCENCE AND PHOTOVOLTAIC SOLAR CELL APPLICATIONS

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ABSTRACT

The development of new functional materials with cutting-edge electrical and optical properties for optoelectronic applications is encouraged by research on fundamental materials and unique combinations of traditional

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materials, nanostructures with the II–VI group regime in contrast to other materials, chalcogenides stand out due to their use in solar selective coatings, solar cells, photoconductors, solar panels, and several other parts. To produce portable, flexible, and more adaptable nanocomposites, inorganic materials must be incorporated into solar systems. ZnSe/polyvinyl alcohol (PVA) nanocomposites have been used as photoelectrodes to assess plenty of photovoltaic characteristics, such as open-circuit voltage (V_{oc}), short-circuit current (I_{sc}), efficiency, and fill factor, to further investigate the configuration of solar cells incorporating phase change materials. The photoelectrodes were manufactured chemically in the presence of an optically transparent and semicrystalline PVA polymer matrix. The major techniques applied to extensively investigate the ZnSe/PVA nanocomposites were X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV–Vis absorption spectroscopy. Optical and structural evaluations confirmed that the nanocomposites featured particles with an average size of within 3.5 nm. The UV–Vis imaging exhibited a broadband band gap of 3.5 eV for the ZnSe/PVA nanocomposites. SEM imaging of the polymer matrix provides the observation of ZnSe nanocrystals in a structure of nanoflowers. These nanocomposites could possess a greater impact if employed as components for photovoltaic solar cell applications.

18.1 INTRODUCTION

Fabrication of various nanostructures with extraordinary electrical and optical properties is currently the subject of extensive research. The band gap of chalcogenides, for instance of a covalently linked semiconductor material, generally varies from 1 to 3 electron volts (eV), depending on the exact composition. Zinc selenide, one of the available semiconductor nanostructures, has been chosen as a viable component for several device applications. Examples of these applications include photovoltaic cells, laser displays, thin film transistors, light-emitting diodes, optical filters, and sensors [1–3]. The II–VI group of semiconductor particles might have been established using polymers as the host matrix for nanocomposites. These particles have variable diameters and lowered crystallinity. Incorporating these particles into polymers acts as an incentive in terms of protection owing to their content tends to be considerably lower than that of the polymer, creating thick conditions that successfully shield. Researchers are paying increasing attention to polymer-based photovoltaics, which might lead to advancements in the understanding of how these devices perform and how to enhance their efficiency. Polymer nanocomposites have acquired major research importance due to their outstanding physical and chemical properties for a wide range of applications, including biological, optoelectronic, and photonic devices. In these nanocomposites, the polymer layer serves as a buffer, making certain uniformity in the size of the nanocrystals [4, 5].

Due to their specific physical and chemical characteristics, significance in several applications, and other variables doped polymers have received a great deal of attention. By analyzing the linear and nonlinear optical properties of nanocomposites formed with semiconductor NPs embedded in a polymer matrix with those formed with virgin polymer, it would be allowed to change the highlights of the nanocomposites [6]. polyvinyl alcohol (PVA) was deliberately chosen for this study above other polymers because of its optical characteristics, physical characteristics, efficiency in creating films, and biocompatibility. A lot of curiosity has been created by the elements of the II–VI group due to their potential in several optoelectronic devices [7]. These substances frequently exhibit strong radiative recombination, high absorption coefficients, and band gaps that nearly replicate the solar visible spectrum. Semiconductors in the II–VI group have grown more and more attractive as potential materials. Zinc selenide (ZnSe), an element of the II–VI group, is especially encouraging for photovoltaic applications because of its increased solar spectrum absorption and greater photocorrosion resistance [8, 9].

In recognition of their potential in several optoelectronic devices, the elements of the II–VI group have attracted a lot of interest. These materials are frequently identifiable by their strong radiative recombination, high absorption coefficients, and band gaps that closely mimic those of the sun's visible spectrum. The II–VI group of semiconductors has become more and more beneficial as potential materials. Zinc selenide (ZnSe), an element of the II–VI group, is especially encouraging for photovoltaic applications because of its increased photocorrosion resistance and improved solar spectrum absorption [10–12].

Despite a great deal of effort in the creation and investigation of optical nonlinearity in nanoparticle/polymer hybrid materials, it is still challenging to make size-tunable nanoparticles using the proper stabilizers. The application-specific nanocomposites still have space for improvement in terms of nonlinear properties and stability.

Solution-grown polymer–zinc selenide nanocomposites are made in the current investigation in a single step at room temperature. As a result, samples were checked for structural and optical characterization making use of methods such as X-ray diffraction (XRD), scanning electron microscopy

(SEM), and UV–visible spectroscopy. The ZnSe/PVA nanocomposites are furthermore employed as a photo-electrode for photovoltaic research according to photoelectrochemical (PEC) cell engineering.

18.2 MATERIAL AND SYNTHESIS

18.2.1 MATERIAL

Analytical-grade sodium selenosulfate (Na_2SeSo_3), zinc chloride ($ZnCl_2{\cdot}2H_2O$), and PVA were incorporated for the synthesis of the ZnSe/PVA nanocomposite. Zinc chloride was decided on as the metal ion, sodium selenosulfate contributed the selenium, and PVA acted as a stabilizing agent. Double-distilled water was utilized as the preparation solvent. It is important to note that all of the compounds used were of analytical quality.

18.2.2 SYNTHESIS

The thin layer of ZnSe/PVA nanocomposite was created utilizing a readily available chemical procedure. The Se source was 100 ccs of sodium sulfite in water (1M), which was produced. The resultant mixture was first heated at 60°C to dissolve the selenium in the solution, and then 0.1 mol of selenium powder was added while the liquid was still being rapidly stirred. After using filtration techniques, a sodium selenosulfate solution has been produced.

Distilled water was chosen as the solvent to create 0.1 M of $ZnCl_2$ solution. The creation of a viscous luminous solution involved spinning 3 g of PVA continuously in 50 ml of distilled water at 90°C. To create a nanocomposite of ZnSe and PVA, add 20 ml of PVA repeatedly while also adding 1 ml of each $ZnCl_2$ and Na_2SeSO_3. The mixture was continuously swirled while ammonia was added as a complexing agent to raise the pH to 10. After swirling for 90 minutes, ZnSe/PVA nanocomposites materialized. The size of the nanocrystals was determined by the polymer matrix's presence.

After that, a glass substrate was coated with the liquid containing the nanocomposite. A thin layer of ZnSe/PVA nanocomposite evolved when the solvent evaporated. A 1.5-hour annealing treatment at 150°C was used on the successfully constructed nanocomposite film. This annealing technique was used to make it better for assessing photovoltaic parameters in PEC cells.

18.2.3 CHARACTERIZATION

The Bruker AXS D8 Advance diffractometer with a Cu X-ray source, wavelength 1.506, was used at SAIF Cochin STIC to record the XRD pattern for structural investigation. In order to analyze the surface morphology of an annealed sample, an SEM-EDS model with the specifications JEOL Model JSM-6390LV and JEOL Model JED-2300 was used at SAIF Cochin STIC. With the use of a PC-based double-beam UV–Vis Spectrometer [Type 2201], optical absorption spectra were captured.

18.2.4 PEC CELL CONFIGURATION AND EXPERIMENTAL SETUP FOR PHOTOVOLTAIC PARAMETER MEASUREMENT

It is important to use a material acceptable for a photoanode and/or a photocathode when building a PEC device for water splitting. Solar energy can be used by PEC cells to create hydrogen; however, their efficiency is much lower in this situation. The chemical process that converts water into hydrogen (H_2) and oxygen (O_2) is particularly carried out by PEC cells using light energy (photons). In this battery, the cathode and anode are submerged in an electrolyte and linked to an external circuit. One of the electrodes (cathode or anode) is often a semiconductor that can absorb sunlight, and the other electrode is often a metal. When photons with energies bigger than the semiconductor’s band gap are absorbed, electron–hole pairs appear in the space charge region between the semiconductor and the electrolyte. An electric field is subsequently used to separate these electron-hole pairs.

In order to reduce extra light absorption, one vessel must be painted black before the ZnSe/PVA nanocomposite photoelectrode is deposited on a titanium substrate and used as a photoelectrode. Graphite is then used as the counter electrode. The polysulfide solution made by combining the aforementioned ingredients with 30 cc of distilled water and letting them dissolve for 24 hours serves as the electrolyte in the PEC cell assembly. Details are provided in Table 18.1.

TABLE 18.1 Electrolyte Composition for PCM Cell Configuration ⏎

Chemical	**Sulfur (S)**	**Sodium Hydroxide (NaOH)**	**Sodium Sulfide (Na_2S)**
Quantity	1M	1M	1M

18.3 RESULT AND DISCUSSION

18.3.1 X-RAY DIFFRACTION STUDIES

Figure 18.1 shows the XRD pattern of the ZnSe/PVA nanocomposite. Using this pattern, other research has been carried out, such as the investigation of hkl planes, interplanar distances, cell size, and lattice parameters. The ZnSe/PVA nanocomposite's diffraction peaks at 2=19.672°, 20.494°, 27.824°, 32.130°, 34.444°, 39.203°, and 45.785°, respectively, are used to demonstrate the (100), (110), (111), (200), (210), (211), (220), and (300) planes. The nanocomposite's crystalline structure is what gives rise to these diffraction peaks.

Since the XRD pattern in Figure 18.1 displays a distinct diffraction peak at around 2θ=19.672° (within the range of 19°–20°), PVA may be semicrystalline. This unique peak at 19.6° [13] of PVA monomer units indicates strong intramolecular hydrogen bonding as well as intermolecular hydrogen interactions between one another. A distinctive diffraction angle that was seen at 2 (SAIFXR150914C-15) can be used to identify ZnSe. The diffraction peaks corresponding to the (111) plane confirm the predominant orientation of the ZnSe nanoparticles, which is the face-centered cubic (fcc) crystal structure. The Debye Scherrer formula was used to determine the crystallite size of the ZnSe/PVA nanocomposites by analyzing the broadening of the diffraction peaks [14].

$$D = \frac{k\lambda}{\beta\cos\theta} \tag{18.1}$$

The essential equations characterize the X-ray wavelength used (= 10540), full width at half maximum (FWHM) of the intensity of the diffraction peak, *k* the wave vector, *D* the size of the crystallite, and the Bragg angle. The wide peaks of the diffraction pattern represent small particles or crystallites with sizes close to 3.5 nm. Peak widening may be caused by particle size restrictions or material faults such as sample-specific residual stress. The lattice constants estimated using the highest-angle reflection data are usually accurate; however, there is a difference for different sample orientations. We determined the ZnSe nanoparticles' lattice constant using the distance-based Nelson–Riley method.

18.3.2 MORPHOLOGICAL STUDIES

In Figure 18.1, a full analysis of the topography of the ZnSe/PVA sample can be obtained from SEM micrographs produced from the SEM-EDS model.

SEM micrographs taken at various magnifications are shown in Figure 18.2. The micrograph reveals how the ZnSe nanoparticles behave specifically to generate a structure like a flower with a limited size distribution. This finding supports the idea that crystallites in ZnSe films containing PVA have a distinct morphological structure. PVA, a stabilizer molecule, attaches to the nanoparticles' surfaces, stabilizing the core and bigger nanoparticles, preventing aggregation, and preventing the growth of nanoparticles up to about 100 nm in size [15, 16].

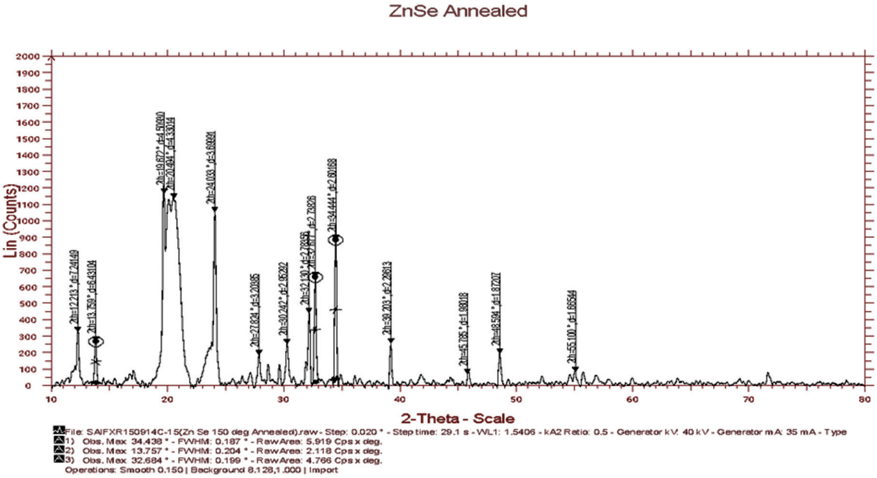

FIGURE 18.1 XRD spectra of ZnSe/PVA nanocomposite. ⏎

18.3.3 OPTICAL ABSORPTION STUDIES

The optical properties of the ZnSe/PVA nanocomposites have been studied using UV–visible spectroscopy. By observing the absorption in the ultraviolet and visible spectra in figures, it is possible to see the transitions between energy levels, particularly the lowest energies of excitons. Using a two-beam UV–Vis spectrometer (PC-based, Type-2201), Figure 18.3 highlights the optical absorption spectra of a ZnSe/PVA nanocomposite film in the 300–900 nm wavelength range. With a decreasing tendency as wavelength increased the prominent edge of the absorption spectrum moved to shorter wavelengths (or higher energies). Such behavior may be shown through zinc selenide's wider band gap. Optical examination shows that the film exhibits a high absorption coefficient and a direct transition type [17].

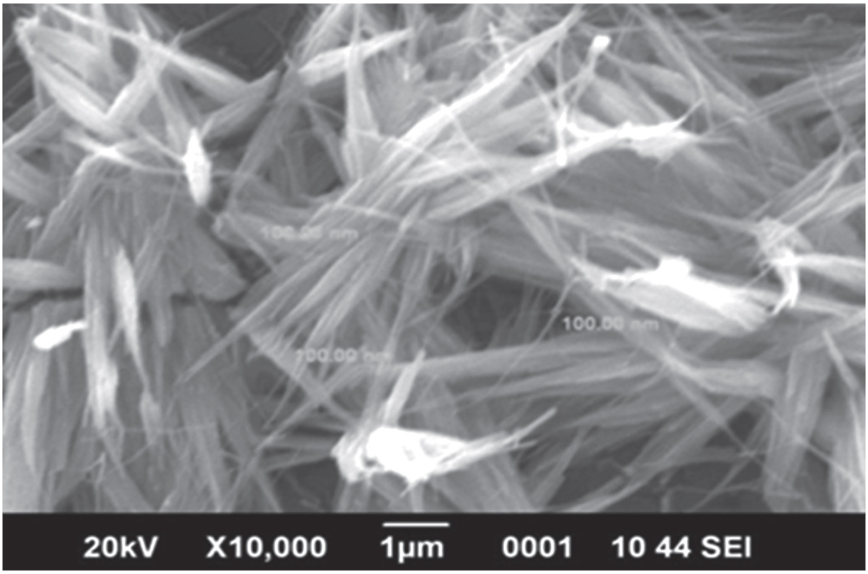

FIGURE 18.2 SEM micrograph of ZnSe/PVA. ⏎

With increasing wavelength, there is a reduction in absorption, and the absorption spectrum shows distinct energy levels with distinct absorption peaks [18, 19]. Thus, it is concluded that higher photon energies are related to shorter wavelengths, whereas lower photon energies are connected with longer wavelengths. The nanocomposite ZnSe/PVA film's band gap was calculated using the equation below:

$$E_{\mathrm{gnano}} = \frac{hc}{\lambda} \tag{18.2}$$

From the band gap information, based on UV–Vis spectra analysis, the particle size of ZnSe/PVA nanocomposite film was estimated by the following equation [20], where h is the Planks constant, c is the velocity of light, and is the absorption edge wavelength of ZnSe/PVA nanocomposite film

$$\hbar = \sqrt{\frac{2\pi^2\hbar^2 E_{gbulk}}{\left(\frac{1}{m_e^*} + \frac{1}{m_e^*}\right)\left(E_{gnano}^2 - E_{gbulk}^2\right) m_o}} \tag{18.3}$$

where r is the particle's radius, m_{e} is the electron's effective mass, m_{h} is the hole's effective mass, E=(E_{gnano}−E_{gbulk}) is the shift in band gap (eV), and m_{o} is the electron's rest mass [21]. Table 18.2 provides the computed values for the band gap, shift in the band gap, absorption edge, and particle size that were obtained from UV–Vis spectra.

TABLE 18.2 Optical Information of ZnSe/PVA Nanofilm by UV–Vis Absorption Spectra

Sample	Absorption Edge Wavelength (λ)Å	Band Gap of E_{gbulk} (eV)	Band Gap of E_{gnano} (eV) from Spectra	Shift in Band Gap ΔE_g in eV	Effective Mass of Electron and Hole of ZnSe/PVA [21]		Particle Size from Spectra in nm
ZnSe/PVA	354	2.701	3.50	0.799	m_e^*	m_h^*	3.51
					0.100	0.160	

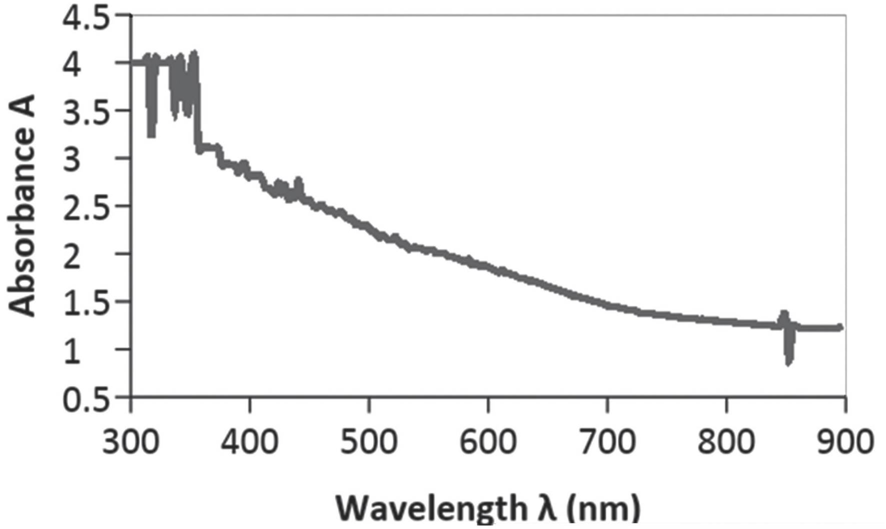

FIGURE 18.3 Absorption spectra of ZnSe/PVA nanocomposite.

18.3.4 PHOTOVOLTAIC STUDIES

The photovoltaic effect is used by a solid-state device known as a solar cell, sometimes known as a photovoltaic cell, to convert light, whether created intentionally or naturally, directly into energy [22]. Nanostructured photoelectrodes have lately gained interest in photovoltaic analysis due to their increased specific surface area and speedier diffusion paths for photogenerated carriers at the interface between the semiconductor and electrolyte. In this study, a ZnSe/PVA nanocomposite was employed as the photoelectrode, and graphite was used as the counter electrode in a PEC cell arrangement. A brief chemical procedure was carried out to synthesize the ZnSe/PVA nanocomposite, which was then coated onto a titanium plate and annealed for 1 h and 30 min at 150°C (Table 18.3). In an electrolyte solution, the working photoelectrode and counter electrode were spaced 1 cm apart [23]. A standard illuminometer (Scientific Laboratory Instrument, Roorkee, Uttarakhand, India) was used to measure the intensity of the illumination offered by a 50 W tungsten lamp placed 10 cm away from the tank, which produced a reading of 315 lux. PEC cell's arrangement for measuring photovoltaic parameters is seen in Figure 18.4. An increase in current appeared after illumination, demonstrating the photoelectric characteristics of the as-synthesized films, and the open-circuit voltage (V_{oc}) was measured in the dark. The ZnSe/PVA nanocomposite's current–voltage characteristics, as determined by adjusting a potentiometer's resistance, are shown in Figure 18.5. Specific formulae were utilized to deduce different solar cell properties from these data, including [24].

TABLE 18.3 Comparison of Band Gap of ZnSe Nanocomposite by Different Techniques ⏎

Authors	Techniques	Band Gap
M. Öztaş et al. [2005]	Spray pyrolysis	2.63–2.70
S. Venkatachalam et al. [2007]	Vacuum evaporation	2.70–2.74
K.R. Murali et al. [2009]	Pulse electrodeposition	2.64–2.68
N.A. Olereke et al. [2011]	Chemical bath deposition	2.70–2.75
S. Anatohe et al. [2013]	Thermal vacuum evaporation	2.70

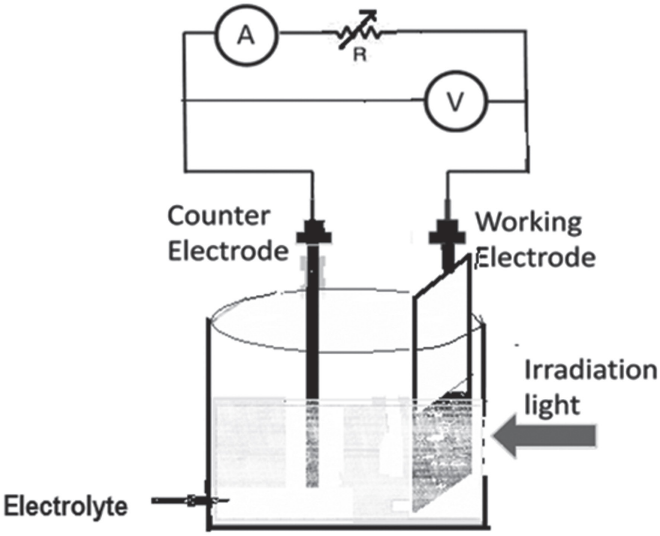

FIGURE 18.4 PEC cell configuration. ⏎

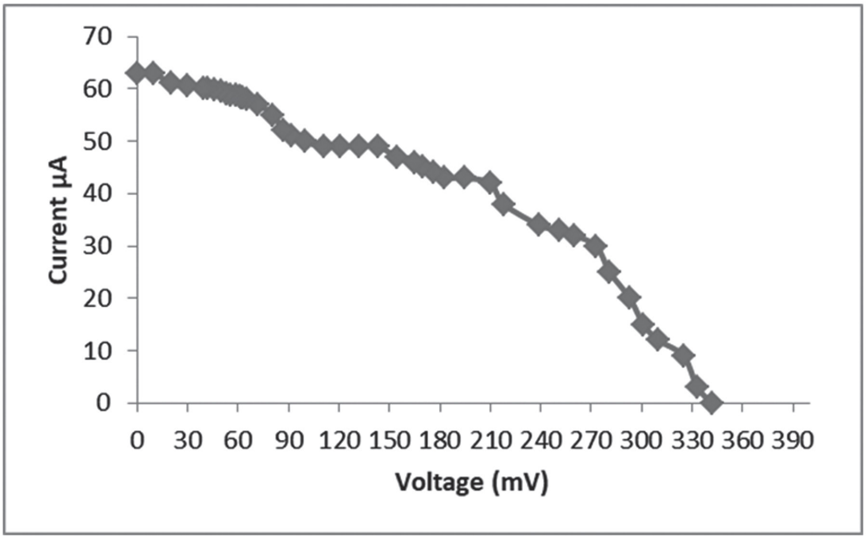

FIGURE 18.5 V–I curve of ZnSe PVA nanocomposites. ⏎

$$\eta = \frac{P_{\text{out}}}{P_{\text{in}}} \rightarrow \eta_{\max = \frac{P_{\max}}{P_{\text{in}}}} \tag{18.4}$$

$$FF = \frac{P_{\text{out}}}{V_{\text{oc}} \times I_{\text{SC}}} \tag{18.5}$$

The measured value of photovoltaic parameters of ZnSe/PVA is given in Table 18.4.

TABLE 18.4 Photovoltaic Parameter Observations ⏎

Sample	Open-Circuit Voltage V_{oc} (mV)	Short-Circuit Current I_{sc} (µA)	Efficiency η	Fill Factor FF
ZnSe/PVA	342	63	3.01	0.139

18.3.5 ELECTROLUMINESCENCE STUDIES

The electroluminescence (EL) studies of chalcogenide nanocomposite (CdZnSe) have been performed. The basic requirements for EL study are given below:

Utilizing a sine/square audio frequency generator, researchers conduct EL investigations in which an aluminum electrode and a conducting glass plate are exposed to alternating voltage at several different frequencies. To generate this voltage and reach high voltage levels, an EL power supply component called a wide band high voltage amplifier (W.B.A.) is used. Subsequently using a photomultiplier tube (PMT) coupled to a pico ammeter, the intensity of EL brightness will be determined over a range of voltage settings and frequencies. A high-voltage power supply produces the 750-volt essential for the PMT to function at that level [25–28]. A precise digital measurement of the intensity of the light being generated is provided by the pico ammeter (Figure 18.6).

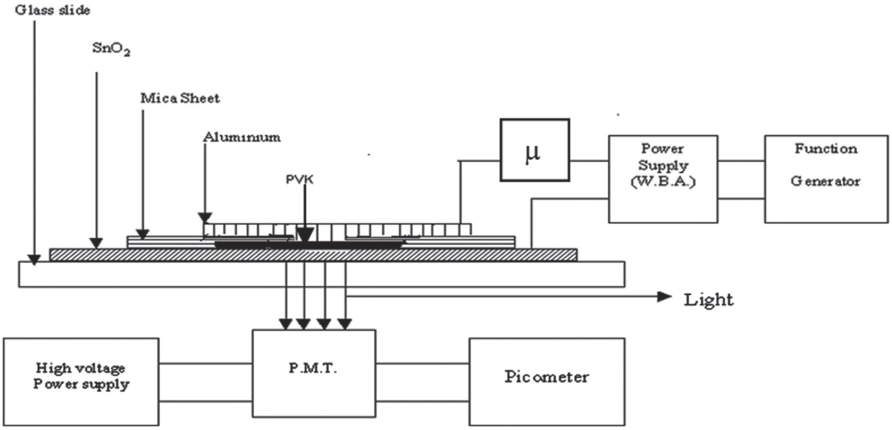

FIGURE 18.6 Setup for electroluminescence study. ⏎

For use in EL research, the function generator's output voltage was initially set at 0.1 V. The input (W.B.A.) of the EL power supply was then linked to this output voltage. The EL cell was then connected to the AC power supply (W.B.A.) and put near to the PMT's aperture. The PMT received 750 V from a power source with an exceptionally high voltage. The output signal from the PMT was then connected to a pico ammeter, which was used to record the PMT's output. EL measurements are set up in the manner as shown in Figure 18.7 [29, 30].

While concurrently monitoring the current and brightness at a specific frequency on the audio generator, the voltage applied to the EL cell was gradually increased. Then, at varied AC voltage settings, the EL brightness for each frequency was measured. Then, we used voltage at various frequencies [31]. To accomplish this measurement, a PMT and a pico ammeter were connected to one another. In addition, we were able to gauge the associated current using an EL cell and a microammeter connected in series.

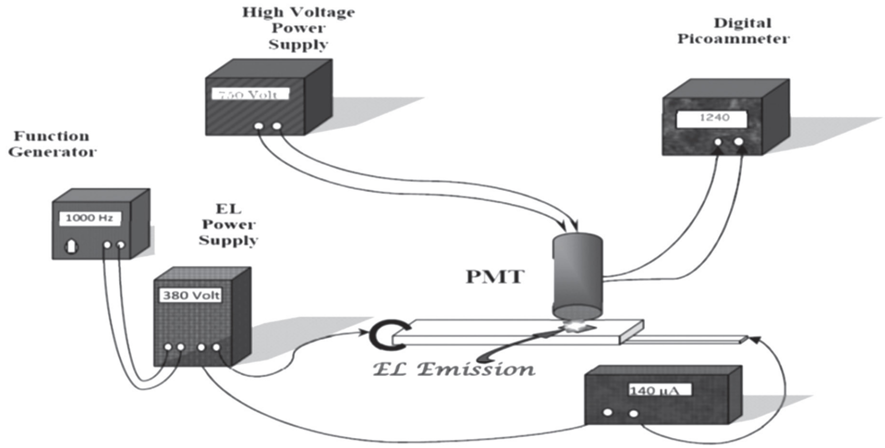
High Voltage Power Supply
750 Volt
Digital Picoammeter
1240
Function Generator
1000 Hz
EL Power Supply
380 Volt
PMT
EL Emission
140 µA

FIGURE 18.7 Arrangement setup for measurement of EL. ⏎

EL spectra were compiled using a grating monochromator and a PMT. The configuration for obtaining EL spectra is shown in Figure 18.8. The grating monochromator's entering slit, which was where the EL cell was located. The monochromator's grating was spun while EL intensity measurements at various wavelengths were being taken. This evaluation was carried out using a PMT placed close to the monochromator's exit slit. Using a digital pico ammeter, the output signal from the PMT was collected and recorded [32].

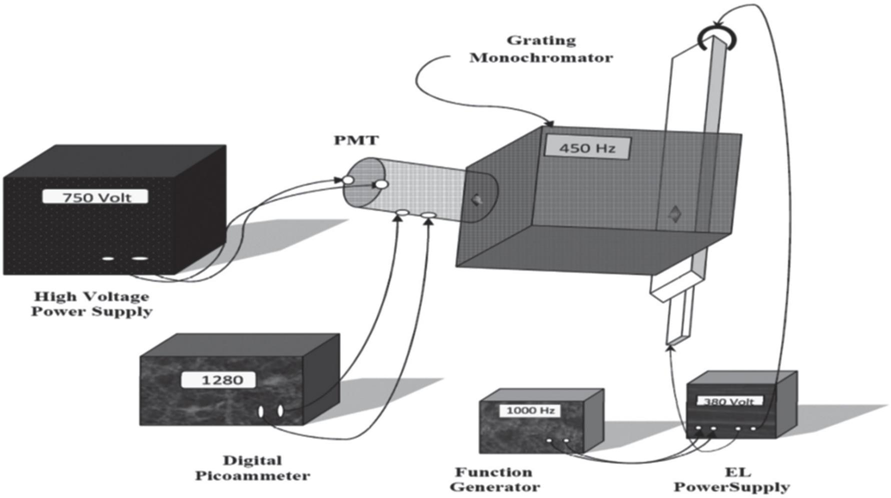
Grating Monochromator
450 Hz
PMT
750 Volt
High Voltage Power Supply
1280
Digital Picoammeter
1000 Hz
Function Generator
380 Volt
EL PowerSupply

FIGURE 18.8 Preparation of electroluminescence cells. ⏎

18.3.5.1 PREPARATION OF ELECTROLUMINESCENCE CELLS

To investigate EL in nanocrystals, a structured layer arrangement EL cell was created. In this configuration, two electrodes are placed between nanocrystal emission layers. One of these electrodes is made to be transparent so that any produced light may be used for practical purposes or for measurement. While the other electrode is normally a metal foil, most often aluminum, the transparent electrode frequently consists of materials like SnO_2 or ITO-coated glass plates.

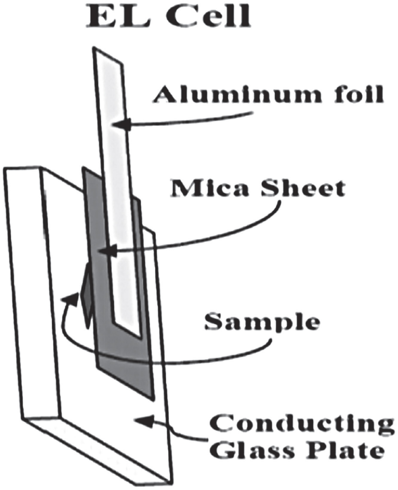

FIGURE 18.9 EL cell. ⏎

The final construction of the EL cell is completed by joining a part of the conducting glass plate with a thin mica sheet that has a small 2×2 mm^2 window. The sample powder was positioned and glued inside of this window. A conducting gel that serves as another electrode is also positioned above the sample location, as seen in Figure 18.9, along with an aluminum strip.

18.3.5.2 FREQUENCY DEPENDENCE OF EL BRIGHTNESS

The frequency response of EL can be explained using the following relationship:

$$N_e = N_{in} (1 - e^{(-t/\tau)})$$

In this equation, N_e represents the number of electrons released from trap states and reaching the conduction band, N_{in} is this value at an infinite time, and τ is the effective time constant for the recombination of charge carriers.

When $t >> \tau$: N_e is approximately equal to N_{in}, signifying a large number of trapped electrons.

When $t < \tau$: N_e is less than N_{in}, indicating fewer trapped electrons.

The acceleration of charge carrier emptying and de-trapping at EL centers makes the frequency dependence of EL brightness simpler. The brightness of EL is found to rise with frequency and occurs at lower threshold voltages at higher frequencies. At higher frequencies, the duration approaches the effective time constant for electron recombination, which equates to a half-cycle of the applied AC voltage. As a result, nonlinearity in the brightness-frequency link may become apparent at higher frequencies.

18.3.5.3 CdZnSe

Starch was utilized as a capping agent at room temperature during the chemical synthesis of $Cd_{1-x}Zn_xSe$ nanoparticles. Five different samples were made, each of which included a different composition component, or "*x*," inside the ternary alloy Cd_{1-x} Zn_xSe. An XRD examination revealed that all of the samples had a cubic crystal structure. The crystallite size ranged from 3 to 9 nm, according to the XRD data, with a clear tendency for size to decrease as Zn content increased in the ternary combination [33].

The lattice constants were also derived from the XRD data, and the Nelson-Reley plot method was used to enhance the accuracy of the findings. The adjusted values closely matched the standard data and tended to approach the lattice constant of CdSe as "*x*" increased from 0 to 1.

The XRD data was also used to estimate the lattice strain, which ranged from 0.023 to 0.026.

It was also shown that the lattice strain and the nano size of the particles both contribute to the broadening of the XRD peak. SEM was used to find particle clusters in the range of a few hundred nanometer. It was discovered that the particle size reduced as the Zn content increased.

The optical absorption spectra showed a discernible blue shift in the absorption edge as Zn content increased. The relationship between absorbance and transmittance as a function of wavelength showed that, with the exception of one wavelength, both values were substantially consistent throughout a wide range of visible light wavelengths. The band gap was established by the examination of absorption, and it was seen that the band gap increased as the Zn level of the compound increased [34].

The greater band gap values in each sample as compared to their bulk counterparts were thought to be the cause of the quantum confinement phenomenon. Photoluminescence (PL) tests were conducted using 410-nm excitation, and a single peak at 445 nm was discovered for the Cd0.25 Zn 0.75Se sample. An emission peak for Cd0.75 Zn 0.25Se moved to 512 nm when "*x*" decreased, resulting in a red shift. This research discovered PL emission that matched band-edge emission.

18.3.5.4 ELECTROLUMINESCENCE

The brightness versus voltage curve, often known as the B–V curve, is frequently used to determine the brightness of electroluminescent materials. This curve shows two crucial properties: the threshold voltage and brightness level. The EL brightness versus voltage curve for several samples at an 800 Hz frequency is shown in Figure 18.10. It is clear that EL emission starts at a specific threshold voltage and increases virtually exponentially as voltage increases.

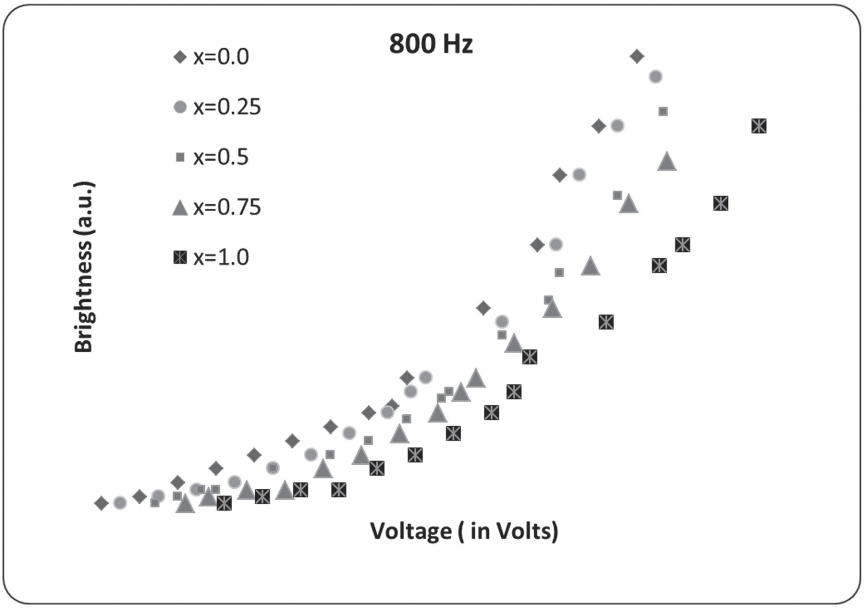

FIGURE 18.10 Brightness–voltage curve for $Cd_{1-x}Zn_xSe$ nanocrystals at 800 Hz. ⏎

In samples with lower Zn concentrations, a reduced threshold voltage and better brightness are particularly noticeable. The recombination of injected electrons and holes from the matching electrodes within the semiconductor nanocrystals is what causes the characteristic light emission in the EL mechanism of semiconductor nanocrystals. The emission layer absorbs more electrons and holes at higher voltages, boosting the brightness of the EL. The stronger oscillators of smaller nanoparticles, which have higher oscillator strength, boost the radiative recombination of electrons and holes. Therefore, the particle size of the same substance may be changed to regulate EL emission [35].

Another crucial element is the ternary nanocrystals' composition. Variations in composition may affect the characteristics of both photoluminescence (PL) and EL.

The relationship between the threshold voltage and the value of "*x*" in Cd_{1-x} Zn_xSe is shown in Figure 18.11. The graph clearly shows that the threshold voltage rises as Zn content in the ternary compound increases.

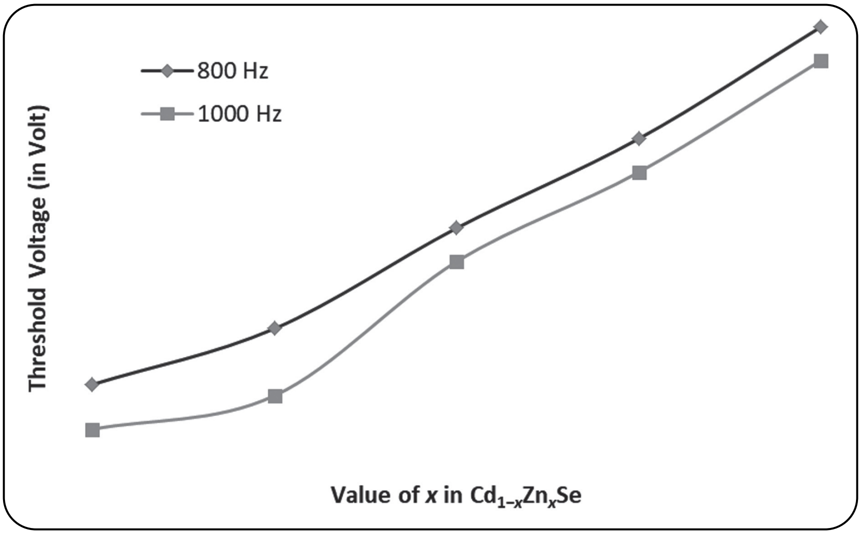

FIGURE 18.11 Effect of *x* on threshold voltage. ⏎

18.3.5.5 FREQUENCY DEPENDENCE OF BRIGHTNESS

Figure 18.13 shows the frequency dependence of EL brightness for $x = 0.25$ samples. Graph between brightness versus frequency at a particular voltage 450 V for all samples is shown in Figure 18.13.

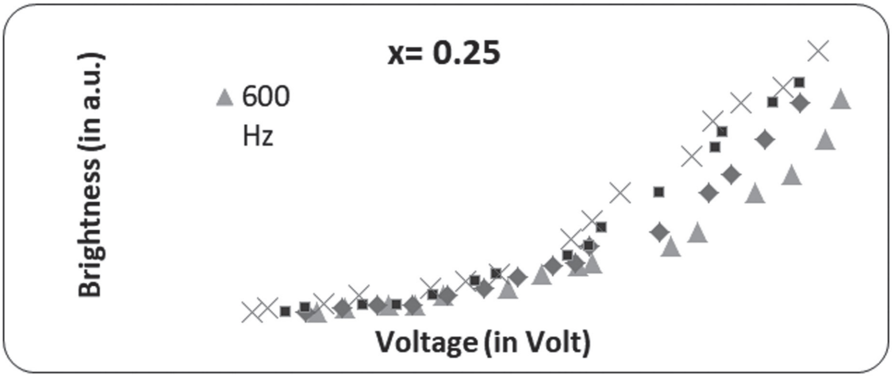

FIGURE 18.12 Voltage brightness curve for Cd0.75Zn0.25Se nanocrystals at different frequencies. ⏎

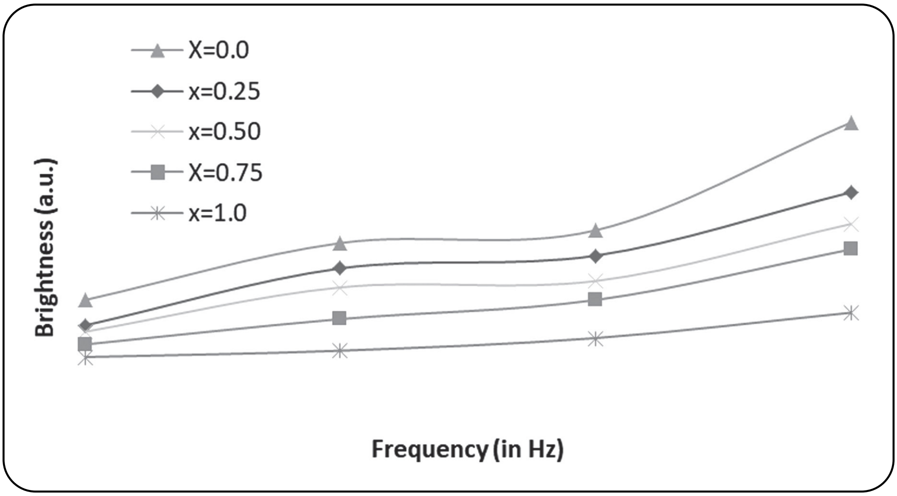

FIGURE 18.13 Frequency dependence of brightness at 450 V. ⏎

Higher frequencies are reported to initiate light emission at lower threshold voltages, while higher frequencies are observed to improve EL brightness.

18.3.5.6 VOLTAGE–CURRENT CHARACTERISTICS

The voltage–current characteristic curves for all five samples are shown in Figure 18.14. It can be observed that the relationship between current and voltage is linear. This demonstrates the ohmic nature, meaning that the electrodes and sample are in ohmic contact. The graphic shows that the slope of the V–I curve falls as Zn concentration in ternary compounds rises. As a result, sample impedance rises. Table 18.5 lists the slope and impedance of several samples [35].

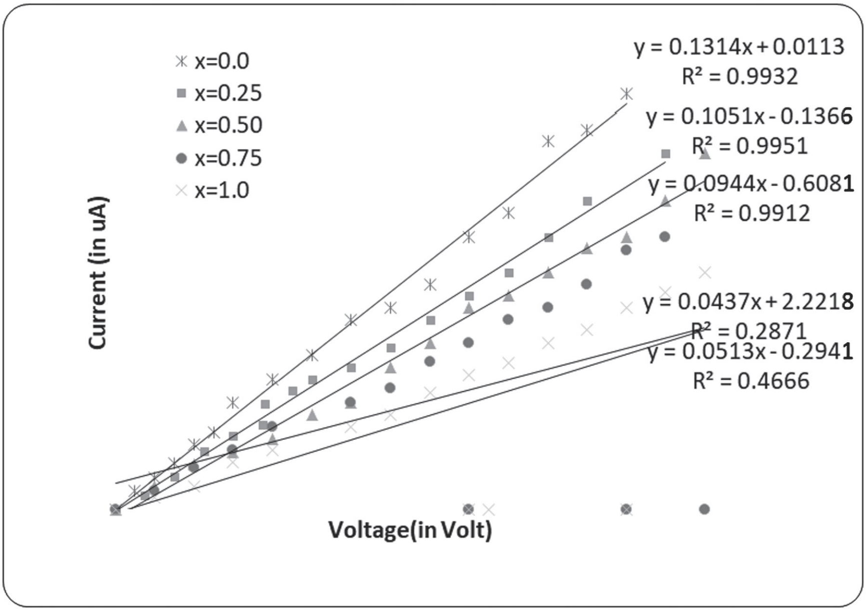

FIGURE 18.14 V–I characteristic curves of Cd$_{1-x}$ Zn$_x$Se at 800 Hz. ⏎

As the composition parameter "*x*" is increased, the band gap of the nanocrystalline films may widen and the grain size may contract, resulting in an overall increase in impedance. Figure 18.15 makes the variation in slope and impedance quite evident.

TABLE 18.5 Composition Dependence of Impedance of EL Cell ⏎

Composition x	Slope of V–I Curve	Impedance of Sample (in MΩ)
0	0.131	7.63
0.25	0.105	9.52
0.5	0.095	10.53
0.75	0.080	12.5
1	0.066	15.15

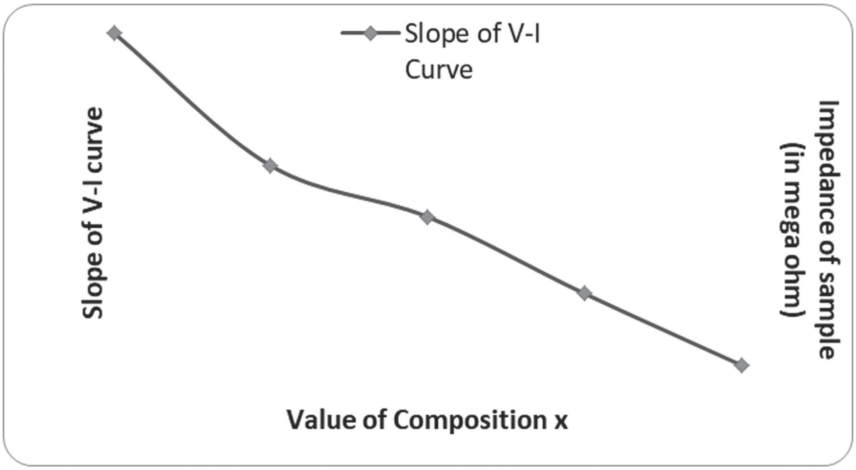

FIGURE 18.15 Composition dependence of slope of V–I curve and impedance of sample. ⏎

Figure 18.16 illustrates the frequency dependence of voltage–current characteristics. The samples exhibit reduced impedance at higher frequencies, as indicated by the slope of the curve rising with frequency.

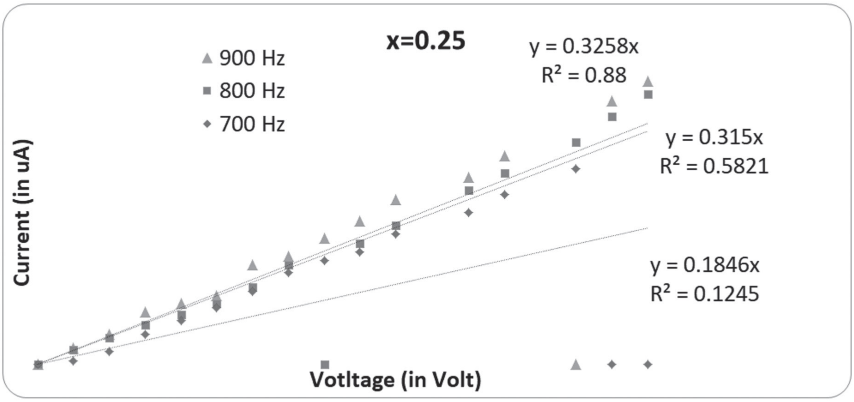

FIGURE 18.16 V–I characteristic curves of Cd0.75Zn0.25Se/PVA at 800 Hz. ⏎

18.3.5.7 SPECTRAL RESPONSE

The EL spectra of $Cd_{1-x}\ Zn_xSe$ nanocrystal (x= 0.25 and 0.5) at 800 Hz are shown in Figure 18.17. For samples with x=0.25 and 0.5, the EL of $Cd_{1-x}\ Zn_x$ Se nanocrystals exhibits emission maxima at 497 and 486 nm, respectively.

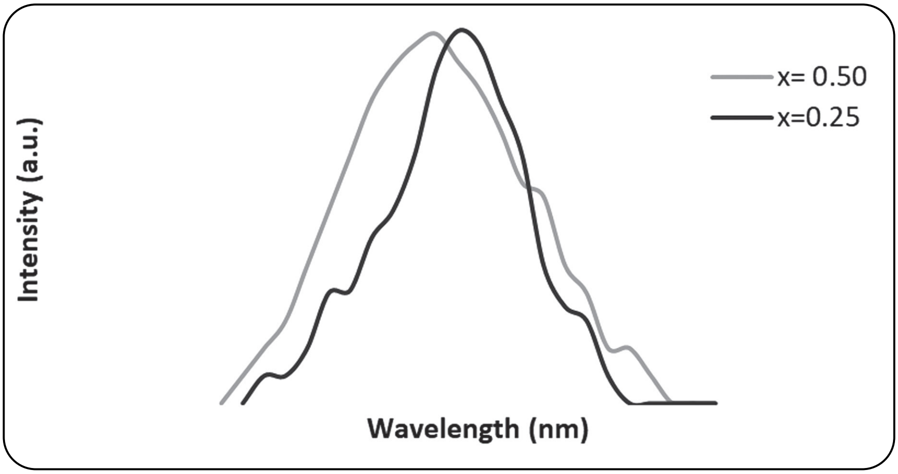

FIGURE 18.17 EL spectra of Cd_{1-x} Zn_xSe nanocrystal samples (x= 0.25 and 0.50) at 800 Hz. ⏎

When we contrast the EL spectra with the results of absorption studies, it is clear that the emission wavelengths almost exactly match the band gap of the samples. The fact that both samples display band-edge emission suggests that the starch may have successfully passivated the surface states. It is important to note that the EL peak has a width of around 50 nm, indicating that certain electronic defect sites may be visible [36–40].

There was a little blue shift in the EL spectra from 0.25 to 0.50 Zn content. This change results from an increase in band gap energy. It is critical to remember that a change in the emission states may lead to a change in the cluster size. Given that the size of Cd_{1-x} Zn_xSe nanocrystals reduces with increasing "x" values in this context, the blue shift in EL may be attributed to fluctuations in the ternary alloy's band gap that are both size-dependent and composition-dependent. These adjustments may alter the state of the material's emissive levels.

18.4 CONCLUSION

We successfully produced ZnSe/PVA nanocomposite films utilizing an eco-friendly one-step solution approach, using PVA as a flexible surfactant, stabilizer, and matrix. Semiconducting nanoparticles can be incorporated into polymeric materials to significantly control a number of crucial material properties, such as nanoparticle size, selenide particle protection from photo-oxidation, nanoparticle aggregation prevention, and photo-induced responses in composites. He carries it out. There was good agreement between the 3.5 nm particle size estimated by XRD and the UV–Vis absorption spectra. However, in 2D or 3D imaging, the particle sizes seen in SEM analysis look bigger (about 100 nm), which can cause clustering of the particles and overestimation of their sizes. For PEC cells, the dense particle packing in the nanocomposite film produces a pinhole-free morphology that enhances the spatial interaction between particles. According to optical research, the highest absorption peak moves to shorter wavelengths, increasing the amount of trapped energy in the process. The band gap (3.5 eV) of the semiconductor nanocrystal effectively rises as a result of a downward valence band shift and an upward conduction band strain. Through photovoltaic investigations, the ZnSe/PVA nanocomposite film's efficiency was calculated to be 3.01%. It may be presumed that ZnSe/PVA nanocomposites are attractive for possible uses in solar devices based on the findings of photovoltaic investigations.

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KEYWORDS

- **II–VI semiconductors**
- **chalcogenides**
- **photovoltaic**
- **XRD**
- **SEM**
- **UV–Vis spectra**
- **photoelectrochemical cell**

REFERENCES

1. Kushwaha, K., Gautam, N., Singh, P., Ramrakhaini, M. Synthesis and photoluminescence of CdSe/PVA nanocomposites. *J. Phys.: Conf. Set.*, **2012**, *365*, 012014.

2. Kushwaha, K., Gautam, N., Singh, P.K., Singh, G., Ramrakhaini, M. Photoluminescence of ZnSe PVA nanocomposite films. *Int. J. Lumin. Appl.*, **2014**, *4*(II).
3. Badr, Y., Mahmoud, M.A. Optimization and photophysics of cadmium selenide nanoparticles. *Phys. B.*, **2005**, *369*, 278–286.
4. Hagfeldt, A., Graetzel, M. Light-induced redox reactions in nanocrystalline systems. *Chem. Rev.*, **1995**, *95*, 49–68.
5. Muntaz Begum, S.K., Rao, M.C., Ravikumar, R. Cu^{2+} doped PVA passivated ZnSe nanoparticles-preparation, characterization, and properties. *J. Inorg. Org. Met. Polym. Mater.* **2013**, *23*, 350–356.
6. Lalwani, G., Henslee, A.M., Farshid, B., Lin, L., Kasper, F.K., Yi, Y.-X., Qin, X., Mikos, A.G., Sitharaman, B. Two-dimensional nanostructure-reinforced biodegradable polymeric nanocomposites for bone tissue engineering. *Biomacromolecules*., **2013**, *14*(3), 900–909. https://doi.org/10.1021/bm301995s.PMC 3601907. PMID 23405887.
7. Kushwaha, K.K., Ramrakhaini, M., Optical studies of CdSe/PVA nanocomposite films. *AIP Conf. Proc.*, **2018**, *1953*, 030099.
8. Gatti, T.; Vicentini, N.; Mba, M.; Menna, E. Organic functionalized carbon nanostructures for functional polymer-based nanocomposites. *Eur. J. Organ. Chem*., **2016**, *2016*(6), 1071–1090. https://doi.org/10.1002/ejoc.201501411. ISSN 1099-0690.
9. Kumari, S., Kumar Kushwah, K., Dubey, S., Ramrakhiani, M. Studies on CdSe/PVK nanocomposites films for electroluminescent display applications. *Opt. Mater.,* **2019**, *97*, 109319.
10. Singh, B.P., Singh, D., Mathur, R.B., Dhami, T.L. Influence of surface modified MWCNTs on the mechanical, electrical, and thermal properties of polyimide nanocomposites. *Nanoscale Res. Lett*., **2008**, *3*(11), 444–453. https://doi.org/10.1007/s11671-008-9179-4
11. Hambrock, J., Birkner, A., Fischer, R.A. Synthesis of CdSe nanoparticles using various organometallic cadmium precursors. *J. Mater. Chem*., **2001**, *11*, 3197–3201.
12. Firth, A.V., Haggata, S.W., Khanna, P.K., et al. Production and luminescent properties of CdSe and CdS nanoparticle polymer composites. *J. Lumin.*, **2004**, *109*, 163–172.
13. Ravindranadh, K., Shekhawat, M.S., Rao, M.C. Preparation and applications of ZnSe nanoparticles. *AIP Conf. Proc.*, **2013**, *1536*, 219–220.
14. Alagumuthu, G., Kumar, T.A. Structural, optical and photocatalytic activity of polymer capped zinc selenide nanoparticles. *Int. Res. J. Eng. Technol. (IRJET)*, **2016**, *03*(11).
15. Phukan, P., Saikia, D. Optical and structural investigation of CdSe quantum dots dispersed in PVA matrix and photovoltaic applications. *Int. J. Photoenergy*, *2013*, 6, 728280.
16. Turner, J.A., et al. *Photoelectrochemical water systems for H_2 production*. National Renewable Energy Laboratory, 2007. Retrieved 2011-05-02.
17. Gautam, A., Ram, S. Preparation and thermomechanical properties of Ag PVA nanocomposite films. *Mater. Chem. Phys.*, **2010** *119*, 266–271.
18. Hammond, C. *The basics of crystallography and diffraction*. Oxford University Press: Oxford, 1997.
19. Guinier, *X-Ray diffraction*. Freeman: San Francisco, CA, USA, 1963.
20. Celine Rose, I.R., Michael Raj, F., Sathish, R., Jeya Rajendran, A. Structural, optical, dielectric and photovoltaic application of Mn-doped zinc selenide nanoparticle. *J. Chem. Pharm. Sci.*, **2015**, *11*, 43–46.
21. Sperling, R.A., Parak, W.J. Surface modification, functionalization and bioconjugation of colloidal inorganic nanoparticles. *Phil. Trans. R. Soc. A*, **2010**, *368*, 1333–1383.
22. Rinson, M.E., Martinez, M.W., Mirand-Hernandez, M. *Sol. Energy Mater. Sol. Cells*, **2003**, *77*, 25.

23. Rosseti, R., Ellison, J.L., Gibson, J.M., Brus, L.E. *J. Chem. Phys.*, **1985**, *82*, 532.
24. Arthur, E., Lucky, A. Synthesis and characterization of CdS and CdSe quantum dots by UV-VIS spectroscopy. *J. Emerg. Trends Eng. Appl. Sci. (JETEAS)*, **2013**, *4*(2), 273–280.
25. Ameri1, M., Fodil, M., Zahra Aoumeur-Benkabou, F., Mahdjoub, Z., Boufadi, F., Bentouaf, A. Physical properties of the ZnxCd$_{1-x}$ Se alloys: Ab-initio method. *Mater. Sci. Appl.*, **2012**, *3*, 768–778
26. Markvart, T. *Solar electricity*. Wiley, 2000.
27. Doug, L. Electronics components: diodes. *Electronics all-in-one desk reference for dummies*. John Wiley & Sons, 2013. Retrieved January 4, 2013.
28. Kushwaha, K., Shukla, P., Nandini, D., Singh, P. Mramrakhiani, electroluminescence from CdSe/PVA nanocomposites. *Nano Vision*, **2011**, *1*, 64–67
29. Kushwaha, K.K., Tiwary, S.K., Vishwakarma, N., Choudhary, Y. Doping of metal precursors on cadmium selenide quantum dots—a review. *J. Nanosci. Nanoeng. Appl.*, **2017**, *7*(3).
30. Kushwaha, K.K., Kumari, S., Mahobia, S.K., Tiwary, S.K., Sinha, B.K., Ramrakhiani, M. Synthesis and characterization of ZnSe/CdSe/ZnS nano-particles embedded in polymer matrix: a review. *IJJCM* **2018**, *4*, 28–33.
31. Gupta, S., Kumar, A., Mukherjee, S., Kumar Kushwah, K., Kumar Mahobia, S., Patharia, P., Kushwaha, A., Yadav, D., Dwivedi, U.K., Kumar, S., Kant Choubey, R. Temperature-dependent study of the fabricated ZnS/p-Si heterojunction. *Physica B: Condens. Matter*, **2023**,*657*(15), 414831
32. Vishvkarma, N., Kushwaha, K., Saxena, V., Khare, K. Morphological and optical properties of pure and doped ZnS nanoparticles: a review. *J. Nanosci. Nanoeng. Appl.*, **2018**, *8*, 1–4.
33. Gautam, N.K., Kuraria, S.R., Kushwaha, K. Kuraria, R.K., Ramrakhiani, M. Electroluminescence in Cd$_{1-x}$ Zn$_x$S nanocrystals. *Int. J. Lumin. Appl.*, **2014**, *4*, 14–16
34. Kushwaha, K.K., Ramrakhaini, M. Optical studies of CdSe/PVA nanocomposite films. In *AIP Conference Proceedings*, 1953, Vol. 30099
35. Kushwaha, K.K., Singh, P.K., Ramrakhiani, M. Photoluminescence studies of cadmium selenide polymer-nanocomposite films. *Int. J. Lumin. Appl.*, **2015**, *5*, 454–455
36. Kumari, S., Kushwaha, K.K., Sahu, P.D., Ramrakhaini, M. Synthesis and electroluminescence in CdSe nanocrystals. In *AIP Conference Proceedings*, 2019, Vol. 2142
37. Kushwah, K.K., Gupta, N., Khare, K., Singh, S., Aziz, F., Ramrakhiani, M. Synthesis and characterization of ZnSe/PVA nanocomposites for optical devices. *Adv. Electromagn.*, **2019**, *8*, 44–49.
38. Hiran, K., Khazanchi, K., Kumar, D., Vyas, A., Padmanaban, S. *Machine learning for sustainable development*. De Gruyter: Berlin, Boston, 2021. https://doi.org/10.1515/9783110702514
39. Vyas, A.K., Balamurugan, S., Hiran, K.K., Dhiman, H.S. (Eds.), *Artificial intelligence for renewable energy systems*. John Wiley & Sons, 2022. ISBN: 9781119761693
40. Singh, S., Kumar Arya, R., Sahana, B.C., Vyas, A.K. (Eds.), *RF circuits for 5G applications: designing with mm wave circuitry*. John Wiley & Sons, 2023.

INDEX

A

Active Learning Algorithm, 179–180
Active origami, 374
active property tuning (APT), 34–35
active smart materials (ASMs), 5–6, 15, 58
active strain energy tuning (ASET), 34–35
actuating systems, 29–30
  thermo-responsive materials, 30–35
actuators, 12, 135, 320–323
  advantages, 324
  CNT-based, 275
  material classes, 59
  piezoelectric, 15
  SMA-based, 324
  types, 325–326
actuator-sensor synthesis, 324–327
additive manufacturing (AM), 100, 269–271, 360
advanced materials, 4
Ag-Cd-based SMAs, 317
alginate, 209–210, 215
alginate/pNIPAM ICE gel inks, 365
alkaline solution, in geopolymerization, 251
aluminum, 271, 273
amorphous silicon thin film (a-Si) solar cells, 350–351
α-amylase, 207
β-amylose, 207
annealing, 9
articulated robots, 277
artificial intelligence (AI) systems
  coating material, 131–132
  designing innovative surface materials and image analysis, 132–133
  integration with digital twin systems, 164
Artificial Neural Network, 176
atomization, 9
austenite, 30, 383–384
austenite phase, 6–7, 10–12
austenite to martensite transformation, 10
AutoCAD, 281
automated guided vehicles (AGVs), 277
automated unmanned machines, 269
autonomous mobile robots (AMRs), 277
azobenzene polymers, 149

B

barbituric acid (Ba), 230
  as acceptor unit, 234
Behler-Parrinello Neural Net, 185
benefit robots, 268–269
beta-1,3/1,6-glucan, 216
big data, in materials science, 127–128
  compound identification using genetic algorithms, 128–129
  data sharing and molecular modeling, 127
  scientific research, 128
  use of chemical and biological sensor networks, 131
biomedicine, 382–383
biopolymeric nanocellulose, 220
biopolymeric smart materials, 216
biopolymers, 215–216, 219–220
biorobots, 372
bismuth sodium titanate (BNT) nanostructures, 103
bismuth telluride (Bi_2Te_3), 149
blast furnace slag (BFS)/ground granulated blast furnace slag (GGBFS), 244
Blender, 281
blue-shifted dyes, 233
boost converter, 342–343
Bronze Age, 4, 54
Buck converter, 342

C

cadmium telluride (CdTe) solar cells, 351
calcium aluminate silicate hydrate (C-A-S-H) gel, 245, 255
calcium-based additives, 247
calcium-rich aluminosilicate gel, 247
carbazole, 231

carbazole-thiophene-naphthalimide,
  photovoltaic performance analysis, 237
carbon allotropes, 75
carbon fiber composite plastic, 281
carbon fiber-reinforced polymers (CFRPs),
  293, 306–307, 309
carbon fibre, 271
carbon nanomaterials (CNM), 56
carbon nanotubes (CNTs), 274–275
carboxy methyl cellulose (CMC), 208
casting process, 8
cellulose-based bioformulations, 220
cellulose fibers, 216
cellulose nanofibers (CNF), 221
ceramics, 4, 54
chalcogenide nanocomposite (CdZnSe), 413
chemical modification, 115
chemical vapor deposition (CVD), 77,
  102–103, 105, 108, 112–113
chitosan, 212–213
chitosan-based nanoparticles, 217
$CH_3NH_3PbX_3$ perovskite organo-lade halide
  materials, 87
chromic materials, 17, 54
  electrochromic materials, 18
  magnetochromic materials, 18
  photochromic materials, 17
  pH sensitive materials, 19
  piezochromic materials, 18–19
  thermochromic materials, 18
CNT-based artificial muscle tissue, 275
coating material, 42
  artificial intelligence (AI)-based, 131–132
cobots, 272, 278, 285
cold working, 9, 100
collaborative robots or cobots, 269
compensation function, 191
component-focused design, 190–191
Composites Sequencing Program, 173
computational inputs, 124–125
conductive polymers, in EV, 298
copper–aluminium–nickel alloy system, 7
copper indium gallium di-selenide (CIGS)
  solar cells, 351
co-precipitation method, 105
cosmetics industry, NBSMs in, 219–220
coumarin, 229–230
crystal structure prediction, 182–184
Curie, Jacques, 35
Curie, Pierre, 35
customary SMA systems, 317
Cu-Zn-Al nanowires, 100
Cu-Zn-Sn SMAs, 101
cyanoacetic acid (Cy), 230
  as acceptor unit, 234–235

D

damping capacity, 12
DC–DC converters, 342–344
decision optimizer, 180
deep generative models (GMs), 124
deep learning (DL), 171–172
  algorithms, 176
  applications, 172–173
  approach for property linkage, 188
  benefits and drawbacks, 173–175
  component-focused design, 190–191
  crystal structure prediction, 182–184
  degradation detection, 190
  essential elements and ideas, 176–181
  force-field neural network structure using,
    184–185
  in informatics, 181–194
  interpretability of models, 182
  long-term effects, 196
  mesoscale modeling, 193–194
  microstructural design using, 188–189
  for mining structure property, 186
  multiresolution homogenization and
    localization links, 186–187
  spectral models, 191–193
deep learning (DL) algorithms, 124
Deep Learning Network, 176, 178
Deep Learning Neural Network, 180
deep reinforcement learning, 179–180
deep transferable learning-based method, 188
degradation detection, 190
digital twin technology, 144–145
  applications, 145, 150
  case studies, 157–159
  challenges and future directions, 160–164
  definition, 149–150
  durability, 153
  efficiency and reliability, 153
  impact on accuracy and precision of,
    153–155

- instantaneous monitoring and control capabilities, 155–157, 159–160
- integration of smart materials in, 151–157, 165–166
- interdisciplinary collaboration, 164
- maintenance costs, 153
- models, 164
- real-time monitoring using, 156
- self-healing capabilities, 153
- sensing capabilities, 152–153
- standardization, 164
- sustainability, 164
- types, 150

diode-clamped multilevel inverter (DCMLI), 345
diphenylamine, 229
directed energy deposition (DED), 360
DNA-based hydrogels, 397
donor-π-acceptor model, 230–231
- double acceptor unit, 237

donor-bridge-acceptor (D-π-A) model, 228
donor-π-bridge-acceptor model, 231
double donor-π-bridge-acceptor model, 231
3D printing (3DP), 360–361
drug-encapsulated supramolecular hydrogel, 396
dye-sensitized cell, 87
dye-sensitized solar cells (DSSCs), 79, 84–87, 228–231
- charge transport mechanism, 228
- computational details, 231–233, 236–237
- donor–acceptor interaction, 229–230
- efficiency of, 233
- future scope and limitations, 238
- impact of double-donor units on performance of, 234–236
- photogeneration of an electron, 87
- working of, 229

E

elastic electric cable (EEC), 275
electric vehicles (EVs), 292
- cost, 307
- durability and lifespan of, 306, 309
- energy efficiency, 306
- energy storage capacity of, 308
- future directions for SMs in, 308–309
- integration of materials, 307
- recyclability of vehicles, 306
- regulatory approval, 308
- reliability, 307
- smart materials in, 292–309
- structural integrity of, 309
- thermal management, 308–309
- types of SMs used in, 296–301

electroactive polymers (EAPs), 297
electrochemical deposition method, 106, 113
electrochromic materials, 18
- in EV, 297–298
- fabrication techniques for, 107–109

electrodeposition, 100–101
electroluminescence (EL) studies
- brightness, 414, 416–417
- B-V curve, 418
- of chalcogenide nanocomposite (CdZnSe), 413, 417–418
- frequency dependence of EL brightness, 419–420
- intensity measurements, 415
- preparation of electroluminescence cells, 415–416
- setup for, 414–415
- spectral response, 422–423
- V-I curve, 420–422

electrophoretic deposition (EPD) technology, 103
electro-responsive materials, 366–367
electrorheological fluids, 20, 39–40
electrorheological materials, 54
electrospinning, 114
electrospun nanofibers, 56
electrostrictive materials, 15–16, 36, 54
emulsion polymerization, 114
1,4-β-Endoglucanose, 208
energy storage in EVs, 308
engineered skin, 272
1,4-β-exoglucanose, 208
exoglucanoses, 208
exoskeletons, 280
expert systems, 130

F

fabrication techniques for SMAs
- additive manufacturing, 100
- chemical modification, 115

  chemical vapor deposition (CVD), 102–103, 105, 108, 112–113
  cold-working, 100
  co-precipitation method, 105
  electrochemical deposition, 106
  electrochromic deposition, 113
  of electrochromic materials, 107–109
  electrodeposition, 100–101
  electrophoretic deposition (EPD) technology, 103
  electrospinning, 114
  emulsion polymerization, 114
  hydrothermal method, 106
  hydrothermal synthesis, 103–104
  inkjet printing, 109
  layer-by-layer assembly, 115
  lithography, 103
  melting and casting, 98–99
  microencapsulation, 109
  of photochromic materials, 111–113
  of pH-sensitive polymers, 113–115
  of piezoelectric materials, 101–104
  polymerization, 111
  powder metallurgy, 99
  self-assembly, 110
  of self-healing materials, 109–111
  shape-memory polymers (SMPs), 98–101
  sol-gel processing, 102, 104–105, 107–108, 112
  solution polymerization, 114
  solvothermal method, 105–106
  spin coating, 108, 113
  spray pyrolysis method, 106–107
  sputtering, 108–109
  of thermochromic materials, 104–107
  three-dimensional (3D) printing, 111
FCA-FA-based geopolymer concrete, 247–252
  casting and curing, 252
  compressive strength, 255–258
  effect of excess of MgO, 257
  mineralogical phases, 250
  mixing process, 252
  mixture proportion, 252
  particle size analysis, 250
  properties of, 248–249
  scanning electron microscope (SEM) images of, 251
  scope of future research, 258
  slump test, 254–255
  testing methods, 253–254
  volume of magnesium oxide (MgO), 247, 250
  workability of, 254
  XRD diffractograms of, 251
ferrochrome ash (FCA), 246
ferroelectric materials, 6
ferroic materials, 319–320
first generation (1G) wafer-based silicon crystalline, 349–350
fluorine-doped tin oxide (FTO), 80, 87
fly ash (FA), 246
  incorporated geopolymer samples, 246
flying capacitor inverter (FCI), 345–347
food packaging, 214–215
force-field neural network structure, 184–185
four-dimensional (4D) printing, 360–362
  in active origami, 374
  applications, 370–377
  challenges and future, 376–377
  4D bioprinting, 371–372
  electro-responsive materials, 366–367
  factors responsible for, 362–363
  laws of, 363–364
  magneto-responsive materials, 367
  photo-responsive materials, 366
  responsible factor for, 373
  self-adaptive materials, 369
  in self-evolving structures, 373
  self-repairing materials, 369
  shape change effect (SCE), 365
  in soft robotics, 372–373
  in space missions, 374–375
  techniques, 369–370
  thermo-responsive materials, 365–366
  using hydrogels, 364–365
functionalization, 77
fused deposition modeling (FDM), 360

G

gelatin, 208–209, 219
gelatinization, 207
Generative Adversarial Networks, 178–179
Generative AI, 132
genetic algorithm, 128–129

genetic algorithms, compound identification using, 128–129
genome, 129
geopolymer-based insulation materials, 246
geopolymer concrete, 244
  calcium-based additive in, 247
  CO_2 emissions, 246
  constituents and advantages of, 245
  lime water in mixing process, effect of, 247
glucoamylose, 207
α-glucosidase, 207
β-glucosidase, 208
β-1,4-glycosidic bonds of cellulose chains cleavage, 208
GN-perovskite solar cells (PSCs), 87–88
GO/TiOx electron transport film, 85
gradient descent, 178
graphene, 56, 271
  porous graphene inverse design, 139
graphene (GN)
  as an electron-transport layer (ETL), 84–87
  based solar cells, 75, 80–82
  as charge acceptor solar cell, 82–84
  CVD electrodes, 81
  derivatives of, 76
  2D structure of, 82
  extraordinary basal plane of, 77
  fundamental properties of, 78–80
  nanocomposites, 77–78
  optical transparency properties, 80
  oxide, 76
  redox chemical effect of electrolyte, 87
  resistivity of, 82
  single and multilayer, 82
  transmittance (T) of, 80, 82
graphene quantum dots (GQDs), 76
Graphical Neural Network, 193–194
guar gum, 216

H

H-bridge-based cascaded multi-level inverter (HBCMLI), 348–349
heat treatment, 9
hexapod robot
  flying hexapod mathematical model, 283–284
  holonomic analysis, 284
  plan of, 281
high-temperature SMA (HTSMA), 100
humanoid robots, 277
Hummer's method, 80
hydantoin (Hy), 230
  as acceptor unit, 235
hydrogels, 38–39, 219, 364–365, 384–385
  based targeted drug delivery, 394–399
  DNA-based, 397
  multifunctional, 396–397
  smart, 96
  stimuli-responsive, 395–398
  supramolecular, 395–396
hydrothermal method, 106
hydrothermal synthesis, 103–104
hydroxyethyl methacrylate (HEMA), 113
hyperparameters, 125
hysteresis of electrostrictive materials, 16

I

II–VI group of semiconductors, 404–405
image optimization, 133
immune-modulatory biomaterials, 218
independent robots, 269
indium tin oxide, 80
indoline, 229
initiated chemical vapor deposition (iCVD), 113
inkjet printing, 109
intelligent materials, 29, 96
intelligent systems, 43
inverse piezoelectric effect, 14

K

Kevlar, 271, 273
Koopman's theorem, 233

L

laser powder bed fusion (L-PBF), 100
layer-by-layer assembly, 115
lead magnesium niobate (PMN), 36
lead magnesium niobate-lead titanate (PMN-PT) substrates, 102
lead telluride (PbTe), 149
lead zinc niobate-lead titanate (PZN-PT), 102
lead zirconate titanate (PZT), 36
LEDs, 6

- lightweight materials, 280–281, 292–295, 301
- lignin, 210–211
- liquid crystal elastomers, 149
- lithium-sulfur batteries, 308
- lithography, 103
- LUMO, 230

M

- machine learning for smart material, 124–126
  - algorithms, 124
  - based synthesis predictions, 129–133
  - compound identification using genetic algorithms, 128–129
  - material designs with, 133–139
  - optimization of coating performance using, 134
  - particle swarm optimization (PSO), 135
  - phases of ML paradigm, 134
  - in sensor applications, 130
  - use of chemical and biological sensor networks, 131
- magnetic shape memory alloys, in EV, 298
- magnetochromic materials, 18
- magneto-responsive materials, 367
- magnetorheological fluid (MRF), 65
  - in EV, 297
- magnetorheological fluids, 20, 39–40
- magnetorheological materials
  - applications of, 65–66
  - smart, 205–206
- magneto-rheological materials, 54
- magnetostriction, 37
- magnetostrictive materials, 16–17, 37–38, 54
- Martens, Adolf, 31
- martensite, 30–31, 383–384
- martensite phase, 7, 10
- martensite start temperature, 10
- materials knowledge systems, 187
- mechanical robots, 268–269
- mechanical technology, 268
- medical applications of SMs, 382–383, 385–386
  - acoustic therapy, 394
  - in advancing healthcare, 390–391
  - angioplasty, 387–388
  - cancer treatments, 391–392
  - cardiovascular therapy, 388–389
  - chemo dynamic treatment, 394
  - chemotherapy, 392–393
  - electrodynamics therapy, 394
  - hydrogel-based targeted drug delivery, 394–399
  - molecular targeted therapy, 393
  - nano-antitumor therapy, 394
  - nanogel, 399–400
  - orthodontics, 390
  - orthopedics, 389–390
  - phototherapy, 394
  - preparation for, 386
  - properties of, 387
  - radiotherapy, 393–394
- medical devices, 13
- medical nanorobots, 217
- melting and casting, 98–99
- melt spinning, 9
- mesoscale modeling, 193–194
- metallic nanomaterials, 56
- metals, 4, 54
- microelectrochemical systems, 329–331
- microencapsulation, 109
- microstructural design using deep learning (DL), 188–189
- monocrystalline silicon solar cells, 350
- Monte Carlo simulations of industrial applications, 194
- morphotropic phase boundary-near modified-PZT ceramics, 102
- multicrystalline silicon solar cell, 350
- multifunctional hydrogel, 396–397
- multilevel inverter (MLI), 344–345
- MXNet, 177

N

- nanocrystals, 405
- nanocrystal solar cell, 352
- nanogel, 399–400
- nanostructures, 404
- naphthalene, 229
- nature-based packaging materials, 214–215, 220
- nature-based smart biomaterials (NBSMs), 204
  - in agriculture, 218–219
  - in biomedical applications, 217–218
  - as biomedicine, 218

  in construction technologies, 215–217
  in cosmetic applications, 219–220
  in defense technology, 220–221
  in food packaging applications, 214–215
  need for, 206–214
  shape-memory, 204–205
  types, 204–206
networks of generative adversaries, 178–179
neural network-based controllers, 43
neural networks, 43, 177–179
Newtonian fluids, 39
nickel ferrite $NiFe_2O_4$ (NFO) films, 102
nickel-titanium alloys, 64
nickel-titanium (Ni-Ti) alloy system, 7
NiTi, 31
NiTiAg SMAs, 99
Nitinol, 64
Nitinol alloy system, 31
nitinol alloy system, 7
NiTi (Nitinol) SMAs, 99–100
  wire specimens, 100
nonbiodegradable packaging, problems with, 214
non-Newtonian fluids, 39
normalization, 178, 186

O

one-step magnetron sputtering process, 108
optical fiber-based sensors, 40–42
optoelectronic performance parameters for dyes, 233

P

passive smart materials (PSMs), 58
PEC cell configuration and experimental setup, 407
perovskite solar cell rGS layer, 88
phase change materials (PCMs), 306
phenothiazine, 229
phenotypes, 129
phenyl-C61-butyric acid methyl ester (PCBM), 84, 88
pH intuitive polymers, 55
photochromic materials, 17, 64–65
  applications of, 65
  fabrication techniques for, 111–113
  smart, 205
photoexcitation, 87
photoluminescence (PL), 76
  tests, 418
photomechanical materials, 149
photonics, 136–138
photo-responsive materials, 366
photosensitizer, 235–237
photosensitizers, 229
photovoltaic (PV) setup, 74
pH-responsive polymers, 367–368
pH-sensitive materials, 19, 54, 65
  applications of, 65
pH-sensitive monomers, 114
pH-sensitive polymers
  fabrication techniques for, 113–115
pH-sensitive smart material, 38–39
piezochromic materials, 18–19
piezoelectric actuators, 15
piezoelectric effect, 14
  direct, 101
  inverse, 101
piezoelectricity, 13, 35
piezoelectric materials, 6, 13–15, 35–36, 54–55, 154, 327, 367
  applications of, 62–63
  in EVs, 296
  fabrication of, 101–104
  lead-based, 104
  smart, 205
piezoelectric sensors, 15, 42–43
  applications, 43
  construction, 42
polarization of charges, 35
poly(3-dodecylthiophene), 84
poly(ε-caprolactone)and thermoplastic polyurethane (PCL/TPU) blends, 110–111
poly(ethylene glycol) (PEG), 114
poly(3-hexylthiophene), 84
poly(L-lactide) (PLLA), 114
polymeric nanomedicines, 218
polymerization process, 247
polymer nanocomposites, 405
polymers, 4, 54
  inverse designs, 135–136
  nature-based, 214, 217
polymer solar cell, 352
polyvinyl alcohol (PVA), 405
porous materials, 138–139

portable robots, 280
postprocessing methods, 9
potassium-based solutions, 244
powder metallurgy, 8, 99
predictive modeling, 129–133
  crystal structure prediction, 182–184
principal component analysis, 187
pseudoelasticity, 12
pyroelectric materials, 6
PyTorch, 177

Q

quantum dot solar cell, 74
quenching, 9

R

rapid solidification, 9
recyclability of vehicles, 306
reduced GN (r-GN), 76
reduced graphene oxide (rGO), 76
reduced-graphene scaffold (rGS), 88
regularization, 176, 178
reinforcement learning, 124
renewable energy sources, 74
research-based deep learning, 181
reverse piezoelectric effect, 35
rhodamine-*n*-acetic acid (Rh), 230
  as acceptor unit, 236
rhodanine-N-acetic acid (RH) acceptor unit, 236
Roberts-Austen, Sir William Chandler, 30
robots
  additive manufacturing (AM) procedures, 269–270
  applications, 276
  commitments to businesses, 284–286
  general functioning of, 281
  hybrid type of, 278
  maerials for designing components, 274–275
  materials in designing, 271–274
  mobile and stationary, 275–278
  trends, 278–280
  underwater, 324
rolling, 9
rubber-bodied robots, 272–273

S

second-generation (2G) solar cells, 350
selective laser sintering (SLS), 360
self-adaptability, 369
self-assembled peptides, 395
self-assembly, 110, 368
self-cleaning surfaces, 97
self-evolving structures, 373
self-healing coatings, 303
self-healing materials, 97, 109–111, 154, 298, 309, 376
self-healing polymers, 295
self-repair materials, 369
semiconductor deficiency, 274
semiconductors, 274
semisupervised learning, 124
sensors, 13
  4D printing and, 375–376
  material classes, 59
  optical fiber-based, 40–42
  piezoelectric, 15, 42–43
  smart, 155
sensory structures, 29
shape change effect (SCE), 365
shape-memory (NBSMs), 204–205
shape-memory alloy fibers (SMAF), 34–35
shape-memory alloys (SMAs), 6–8, 32–34, 54, 63, 96, 154, 382–384
  aerospace applications, 327–328
  applications, 12–13, 64, 327–328
  commercial applications, 7
  energy harvesting, 144
  in EVs, 12–13, 296
  examples, 7, 63–64
  manufacturing methods, 8–9
  properties, 10–12
  regaining original shape, 8
  responsiveness, 144
  self-healing property, 144
  versatility and adaptability, 144
shape memory effect (SME), 10
shape memory polymers (SMP), 361
shape-memory polymers (SMPs), 98–101, 110–111
  in EV, 296–297
shape recovery, 31
Si-based PV devices, 74
silicon-germanium alloys, 149

silk, 213–214
  protein derivative, 214
silk fibroin (SF), 213
silk sericin, 213
smart biomaterials, 206, 218, 391
  in defense, 220–221
smart materials (SMs), 4, 13, 54, 292, 314–315, 382–383
  action of, 316
  advantages and disadvantages, 69
  in aerospace engineering, 68
  attributes, 5
  in biomedicine, 382–383, 385–386
  in biomedicine and medical diagnostics, 67
  characteristics, 315
  in civil engineering, 66–67
  classification of, 5–6, 62, 316–320
  commercial applications of, 317–319
  in construction and architecture industry, 216
  control of characteristics, 5
  criteria for classification of, 28–29
  definition, 5
  definition and characteristics of, 145–146
  durability of, 306
  energy efficiency, 306
  energy harvesting, 294
  ferroic characteristics of, 319–320
  functionalities, 4
  for improved vehicle efficiency, 301–302
  interdisciplinary natures of, 60
  key features, 5
  for lightweight components, 294–295, 306
  in mechanical engineering, 67
  medical science application, 67–68
  as microelectrochemical systems, 329–331
  nanotechnology and, 328–329
  nature of, 58–59
  needs of, 56–58
  new types of, 163–164
  in nuclear facilities, 68
  properties of, 59–61
  for safety of vehicles, 302–305
  self-healing capabilities, 295–296
  stealth application, 68
  in structural engineering, 67
  for sustainability of vehicles, 305–306
  thermal management, 295
  thermal mitigation, 68
  types, 6–20, 97–98, 146–149
  types of, 61–66
  waste reduction, 69
smart nanomaterial (SNMs), 55–56
smart sensors, 155
  impact on precision and accuracy, 154–155
  in MEMs, 331
smart textiles, 97
Smart Window, 113
Sn-NiO films, 108–109
sodium aluminate silicate hydrate (N-A-S-H) gel, 245, 255
sodium-based alkaline solution, 244
soft actuators (SA), 372
soft robotics, 372–373
solar cells, 6
solar energy, 337
solar photovoltaic system, 337–338
  automatic selection of algorithm (ASA), 342
  charger, 344
  DC-DC converters, 342–344
  IC algorithm, 341
  incremental conductance flow diagram, 341
  inverter and topologies, 344–349
  I-V characteristics of PV cell, 340
  materials for, 349–353
  maximum power point tracking (MPPT) module, 339–342
  Perturb and Observe (P&O) method, 339–342
  PWM-based strategy of two-loop PI control, 344
  standalone, 338–339
sol-gel processing, 102, 107–108, 112
solid-state reaction process, 102
solution-grown polymer-zinc selenide nanocomposites, 405
solution polymerization, 114
solvothermal method, 105–106
spectral models, 191–193
spectrophotometer, 191
spin coating, 108, 113
spray pyrolysis method, 106–107
sputtering, 108–109
starch, 207

steel-bodied robots, 271–272
stereolithography (SLA), 360
stimulation function, 177–178
stimuli-responsive hydrogel, 395–398
Stone Age, 4, 54
sulfur nanoparticles (SNPs), 215
superconductors, 298–301
superelasticity, 12
supramolecular hydrogel, 395–396
"survival of the fittest" principle, 128
sustainable packaging material, 215
Swarm robotics, 280

T

temperature hysteresis, 11
Tensorflow, 177
thermochromic materials, 18, 64
  fabrication techniques for, 104–107
thermo chromic smart materials, 205
thermoelasticity, 10–11
thermoelectric generators, 149
thermoelectric materials, 149
  in EV, 297–298
thermo-responsive materials, 30–35, 365–366
thin-film solar cell, 74
third-generation (3G) solar cells, 351–353
three-dimensional (3D) printing, 111
transfer learning, 180–181
triphenylamine, 229–230
twinned martensite structure, 10

U

ultrasonic additive manufacturing (UAM), 376
ultra-wear-resistant steel, 272
Undaria pinnatifida microparticles, 219
underwater robots, 324
unsupervised learning, 124

V

vanadium oxide (VOx) nanocrystals, 106
vehicle safety with SMs, 302–305
vehicle sustainability with SMs, 305–306
versatile robots, 268–269
VGG16 network, 188
Villari effect, 37

W

wearable robots, 280
well-crystallized BNT nanofibers, 103
wheat starch, 216
wire drawing, 9
wireless sensor networks (WSNs), 131
WO_3 films, 113

X

xanthan gum, 211–212, 216

Z

ZEISS ZEN Intellesis (ZZI) features, 133
zinc-aluminum alloy system, 7
zinc selenide (ZnSe), 404–405
ZnO micro-thornyballs (ZMTBs)-based piezoelectric nanogenerator, 102
ZnSe/PVA nanocomposites, 406
  characterization, 407
  electroluminescence (EL) studies, 413–423
  materials and synthesis, 406
  morphological studies, 408–409
  optical properties of, 409–411
  PEC cell configuration and experimental setup, 407
  photovoltaic effect, 411–413
  XRD studies, 408